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(71) Applicant *(for all designated States except US)*: UNITED STATES OF AMERICA, represented by THE SECRETARY OF THE ARMY [US/US]; Intellectuel Property Counsel of the Army, Office of The Judge Advocate General, DA, Suite 400, 901 North Stuart Street, Arlington, VA 22203-1837 (US).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: REID, Robert, H. [US/US]; 10807 McComas Court, Kensington, MD 20895 (US). SADEGH-NASSERI, Scheherazade [US/US]; 13600 Straw-Bale Lane, Darnestown, MD 20878 (US). WOLFF, Marcia [US/US]; 9850 Hollow Glen Place, Silver Spring, MD 20910 (US). NAUSS, Jeffrey, L. [US/US]; 142 Martha Lane, Fairfield, OH 45014 (US).

(74) Agent: NORRIS, Jerome, J.; Suite 1250, 1401 New York Avenue, N.W., Washington, DC 20005 (US).

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(54) Title: MODEL FOR TESTING IMMUNOGENICITY OF PEPTIDES

(57) Abstract

Assay methods for determining whether a peptide is likely to be immunogenic are based on a computer modeling of binding to a Class II MHC DR1 receptor. This is confirmed by competitive inhibition binding assays. The peptides are useful for eliciting an immune response for vaccination or the production of antibodies or T-cells.

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# MODEL FOR TESTING IMMUNOGENICITY OF PEPTIDES

## Government Interest

The invention described herein may be manufactured, licensed and used by or for governmental purposes without the payment of any royalties to us thereon.

## Cross Reference

This application is a continuation-in-part of U.S. Patent application Serial No. 08/064,559, filed May 21, 1993, and the present application incorporates U.S. Patent Application Serial No. 08/064,559 in its entirety by reference.

## Field of the Invention:

This invention relates to a means of predicting potential of a peptide for eliciting immune response.

## Background of the Invention:

Among the numerous steps required for an immunological response to occur is the presentation of the antigen by macrophages to the B-cell or T-cell. This presentation is mediated by the Class I and Class II major histocompatibility complex (MHC) molecules on the surface of the cell. The MHC molecules hold antigens in the form of the peptide fragments and together with the receptor molecule on the T-cells, form a macromolecular complex that induces a response in the T-cell. Therefore, a necessary step in an immune response is the binding of the antigen to the MHC.

Recent single crystal X-ray structures of human and murine Class I MHC's have been reported. Analysis of these crystal structures have shown that antigenic peptides lie in the so-called binding cleft for presentation to the T-cell. This cleft is formed by $\alpha_1$ and $\alpha_2$ domains and by $\beta$-strands from each domain forming the floor. Furthermore, the sequence polymorphism among Class I molecules can result in alterations of the surface of the cleft forming different pockets. Peptide side chains may insert into these pockets. Thus, different pockets may interact with different side chains. This implies the mechanism for the peptide specificity of Class I MHC's. Peptides bound to the Class I MHC's in the crystal structures were found to have both the amino and carboxy termini tightly held by the MHC. There were few interactions near the middle of the cleft. Hence the bound peptide is allowed to bend slightly in the center. The observed binding mode helped to explain the apparent partial specificity of peptide sequence and the allowed variation in peptide length found among peptides isolated from Class I MHC's.

The precise mode of binding of peptides to Class II MHC molecules is less clear. While a single crystal X-ray diffraction structure for the HLA-DR1 MHC has been shown, the coordinates have remained unavailable. However, currently available theoretical and experimental results help form a hypothesis that the binding of a peptide to Class II MHC is similar to that observed with Class I. First, it is noted that the Class II binding cleft is structurally similar to

that of Class I. This was concluded based upon a sequence analysis of 26 Class I and 54 Class II amino acid sequences.

Unlike with Class I molecules, self-peptides isolated from murine I-$A^b$ and I-$E^b$, from murine I-$A^d$ and from human HLA-DR1 molecules were found to be varied in size (13 to 25 residues long). The peptides isolated from the murine I-$A^b$ and I-$E^b$ molecules had heterogenous carboxy termini while those from I-$A^d$ and HLA-DR1 had ragged termini at both ends. The varying lengths indicate that the amino and carboxy termini of the peptides were not critical for the binding. One or both termini may protrude from the binding site and be available for further processing. The residues critical for binding were proposed to be at the ends of the peptide as opposed to the center.

Summary of the Invention:

It is the purpose of this invention to provide a method for preliminary screening of peptides for ability to elicit an immune response. Structural homology techniques were used to model a receptor (the Class II MHC is exemplified). This model makes it possible to preliminarily screen peptides for antigenic properties. By modifying the peptide to "fit" into the receptor it is possible to identify methods of rendering non-immunogenic peptides immunogenic.

The preliminary screening of peptides for immunogenicity comprises the steps of (1) creating a molecular model of a receptor followed by minimizing the model created, 2) modeling a peptide to be tested and minimizing the model of the peptide, then testing the

fit of the model of the peptide into the model of the receptor to produce a composite minimized receptor/minimized peptide model. Upon finding an acceptable fit, the peptide may then be screened by a binding assay for actual binding to Class II MHC as a further test for immunogenicity.

It has been found that when the model of the peptide can not be fitted into the model of the receptor, the peptide will lack immunogenicity. While not all peptide models which can be made to "fit" into to model of the receptor will be effective as immunogens, the screening methods of the invention may make it possible to avoid undue biological testing of inappropriate peptides. By using the model, it is also possible to alter peptides to accommodate the receptor. Hence, the invention has both predictive and drug design applications.

Brief Description of the Figures:

Fig. 1 shows the HLA-aw68 $\alpha_1$ and $\alpha_2$ domains with DR1 $\alpha_1$ and $\beta_1$ domains.

Figs. 2-30 are a printout of the minimized coordinates of the receptor.

Figs. 31 and 32 shows the effects of various peptides inhibiting the binding of labeled hemagglutinin in a competitive binding assay.

Detailed Description of the Invention:

In order to understand and better predict peptide interaction with Class II MHC's and as an aid for synthetic peptide vaccine design, a structural homology model of HLA-DR1 molecule was made

using the Class I HLA-aw68 as a reference molecule. For purposes of this analysis, numerous conserved residues were aligned leading to a proposed three-dimensional model for the Class II structure very similar to that of Class I. This model retained the overall conformation of a Class I MHC and agreed with a considerable amount of the published data. Furthermore, peptides shown to bind to DR1 were docked in the binding cleft of the model and analyzed. The results agree with the experimental binding data presented here. Hence, it is shown that the structural homology model reported here is useful for screening Class II MHC functionality.

It had been hypothesized that few peptide residues may be required for binding to DR1. By substituting residues into the influenza hemagglutinin 307-319 T-cell epitope (HA) it had been determined that a single tyrosine at 308 was required for binding. A synthetic peptide with the tyrosine at position 308 and a lysine at 315 was found to bind DR1 as well as the native peptide. Hence, it was concluded that few peptide residues determine the high affinity binding to DR1.

The peptides produced according to the present invention may be used alone or chemically bound to another peptide and/or carrier in order to elicit an immune response. An immune response is elicited by administering a peptide to an animal in an effective dose and by an effective route of administration. Typically the peptide will be administered with an immunologically acceptable carrier. The routes of administration, dosages, times between multiple administrations will be based on the particular peptide and are standard operations of those skilled in the art.

Of particular interest are peptides from pathogenic microorganisms and neoplasms. In such an example, a vaccine may be formed with the peptide and any known immunological carrier and may be administered prophylactically or therapeutically. The immune response may be elicited for a number of reasons other than for prophylaxis or therapy such as increasing antibody production for the harvesting of antibodies, or increasing specific B-cell or T-cell concentration for the production of hybridomas or cellular therapy.

The choice of host animals is limited only to those capable of an immune response. Preferred hosts are mammals, more preferred are humans.

The vaccine may contain plural peptides with each peptide corresponding to the same or different antigens. The peptides may be used unbound or they may be chemically bound to another peptide or an unrelated protein or other molecule. A preferred vaccine preparation contains a plurality of peptides chemically bound to a larger more immunogenic peptide.

The peptide may be adsorbed, bound or encapsulated in a biodegradeable microsphere, microcapsule, larger carrier or a combination of these. The carrier may have a slow or controlled release property thereby releasing the peptide under appropriate conditions and times for enhanced immunization. This is particularly important when administering the peptide orally where stomach acid can degrade the peptide.

Another embodiment of the present invention is to modify the amino acid sequence of a peptide to enhance its immunogenicity. This is done by modifying the natural peptide sequence to bind to

the Class II MHC receptor DR1 with superior binding affinity for a Class II MHC receptor DR1 than the natural peptide sequence. This modified peptide is considered a synthetic peptide. Alternatively, the sequence may be modified to have a greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1.

Many amino acid changes are acceptable in the formation of a synthetic peptide. The changes may be for similar types of amino acids such as leucine for isoleucine or they may be for diverse types such as tyrosine for lysine.

Materials and Methods:

The structural homology model for the DR1 Class II MHC was constructed using the QUANTA molecular modeling package (vision 3.2, Molecular Simulations, Inc., Burlington, MA) with the CHARMM and Protein Design modules. After alignment of the sequences as described below, gaps and loops were energy minimized using 100 steps of steepest descents minimization followed by 100 steps of adopted basis set Newton-Rapheson (ABNR) minimization. Large gaps were closed using a fragment database from a selected set of high-resolution crystal structures. The resulting structure was minimized in vacuo using 1000 steps of steepest descents followed by an additional 1000 steps of ABNR minimization. A distance related electrostatic function was used in all calculations with a dielectric constant of 1.0. Non-bound parameter lists were updated every 20 steps with a cutoff distance of 15.0Å. Non-bonded calculations were performed using a shifted potential function between 11.0Å and 14.0Å. An extended atom set was used with only

polar hydrogen atoms specifically placed. There were no explicit hydrogen bond energy calculations performed.

All peptides were initially modeled using QUANTA in an extended chain conformation and subjected to 500 steps of ABNR minimization. The resulting structures remained essentially in extended chain conformations. Individual peptides were manually docked in several different orientations into the binding cleft region of the minimized DR1 structure. The resulting bimolecular complex was subjected to 5000 steps of steepest descents minimization with non-bonded interactions updated every five steps. After minimization, bound peptides remained essentially in extended chain conformations. The lowest energy complexes for each peptide were selected for further analysis.

The selected peptide and DR1 complexes and the minimized DR1 model were subjected to the following molecular dynamics regimen: 300 steps of heating to 300°K, 600 steps of equilibration at 300°K, and 1100 steps of production dynamics. During this simulation, the DR1 Cα atoms were constrained in their starting positions. All non-bonded interaction parameters were as stated for the minimization procedure. The lowest energy structure during the course of the production dynamics was selected and subjected to the 5000 step minimization procedure described previously with the Cα restraints removed. The resulting structures were used for the binding energy calculations and for hydrogen bonding analysis.

Hydrogen bonds were determined using the QUANTA default parameters. Maximum allowed distances were 2.5Å between a hydrogen and the acceptor atom and 3.3Å between the donor and acceptor atoms.

The minimum angle allowed between any set of atoms forming a hydrogen bond was 90°.

Competitive Inhibition Binding Assay:

HA peptide (the influenza hemagglutinin 307-319 T-cell epitope) was labeled with $^{125}I$. The labeled HA peptides were then allowed to interact with purified DR1 molecules during incubation to allow formation of peptide/DR1 complexes. After incubation, the peptide/DR1 composition was exposed to a native gel for chromatographic separation or passed through a spun column to separate labeled peptide/DR1 complex and free labelled peptide. When unlabeled peptides were added before incubation of labeled HA peptides and DR1, and if the unlabelled peptides had capacity for binding to DR1 simultaneous with $^{125}I$-HA, there was a resultant decrease in radioactive signal associated with the DR1. The extent of this decrease directly related to the binding capacity of the unlabeled unknown peptide.

Structural Homology Model for the DR1 Molecule:

The structural homology model was created, the reference molecule being the crystal structure of HLA-aw68. The HLA-aw68 coordinates and subsequent sequence were obtained from the entry 2HLA in the Brookhaven Protein Data Bank released January 15, 1991, which is incorporated herein by reference. The sequence for the DR1 molecule was for the $\alpha_1$ domain was reported by Klein and for the $\beta_1$ domain, the study reported by Todd et al. (Nature 329, 599 (1987)).

The sequence alignment is based on Brown et al. (Nature 332, 845 (1988)). The complete alignment and numbering scheme for both

are seen in Figure 1. The Class II, $\beta_1$ and Class I $\alpha_2$ domains regions were conserved with some variations at the ends where the two MHC's have different loop regions. The fourth B-strand in the $\alpha_1$ domain of HLA-aw68 (residues 30-38) is disrupted in the DR1 model. Only three residues are in a $\beta$-sheet conformation, probably due to the inserted glycine at position 28 before the strand and the large deletion in the loop region immediately after the strand. The two alpha-helical regions are clearly maintained. Both helices have been observed to be discontinuous in the Class I molecules and are similar in the DR1 model. The $\alpha_1$ domain helix is long and curves from residues 49$\alpha$ to 76$\alpha$ without significant disruption. It is essentially a single continuous helix. However, the $\alpha_2$ helical region is broken into two separate helices as with the Class I molecules. A short helix (52-63) is separated from a longer helix (68-94) by a deformed region without secondary structure. This deformation is more pronounced in the DR1 model as opposed to the Class I molecules due to an insertion.

Influenza Hemagglutinin Peptide with DR1:

The amino acid residues 307-319 of influenza hemagglutinin (Pro-Lys- Tyr-Val-Lys-Gln-Asn-Thr-Leu-Lys-Leu-Ala-Thr) make up a well-documented linear T-cell epitope which has been shown to be HLA-DR1 restricted. With the demonstration that the influenza hemagglutinin epitope (referred to as the HA peptide) binds DR1, it was chosen to be modeled into the binding cleft.

The peptide was initially inserted into the cleft so that Leu 11 HA was in the vicinity of the hydrophobic pocket. This allowed Asn 7 to be near the middle charged and polar groups of the cleft.

The remaining residue of the motif (Lys 2) was near the vicinity of the remaining charged and polar residues at the end of the cleft. The only adjustment to the starting conformation was a slight rearrangement of the terminal peptide proline and Tyr 3 to alleviate obvious bad contacts.

After the energy minimization of the bimolecular complex, the total energy was reduced to 483 kcal/mol. This reduction in energy was accomplished by alleviation of several bad contacts and also be formation of several hydrogen bonds. The sticking feature of this mode is lack of hydrogen bonds in the carboxy terminal half of the peptide. Only one hydrogen bond is identified between the backbone carbonyl group of Leu 9 and the side chain of the $\beta_1$ Asn 77. In contrast, the amino terminal half has eleven identified interactions. Four of these interaction involve the peptide backbone residues Tyr 3, Val 4, and Gln 6. The remainder involve the side chains of Lys 2, Tyr 3, Lys 5 and Gln 6. Interestingly, Lys 5 is involved in more interactions (three) than Lys 2 (only 2). No interactions were observed as anticipated with Asn 7. Instead, it was the glutamine at position 6 donating a hydrogen bond to the $\alpha_1$ Asn 62. No interactions were observed for the amino and carboxy termini.

HA-YK Peptide with DR1:

The binding of the HA-YK peptide (Ala-Ala-Tyr-Ala-Ala-Ala-Ala-Ala-Ala-Lys-Ala-Ala) to the DR1 model was tested. In aligning the peptide in the cleft, it was deemed logical to insert the tyrosine residue into the hydrophobic region of the binding cleft. The lysine would then be in position to interact with the

hydrophilic groups in the other half of the cleft. The resulting peptide orientation is the opposite that used for the HA and the CS3 (defined below) peptides. With the peptide oriented as described, the final docking position for the peptide was unclear. The hydrophobic pocket is quite large, and, at least in this model, could accommodate the peptide tyrosine in a number of positions by sliding the peptide lengthwise through the cleft. However, repositioning the peptide also repositions the lysine. There were primarily two positions for the lysine: one with the lysine inside the cleft and the second with it outside. Of the two positions, the former was the lower in energy by 46 kcal/mol and had the greater number of interactions with the protein (11 vs. 7). Thus, the preferred orientation of the peptide appears to be with the lysine inside the binding cleft region.

CS3 subunit Pilin Peptide with DR1:

The suspected T-cell epitope for CS3 pilus subunit 63-78 (Ser-Lys-Asn-Gly-Thr-Val-Thr-Trp-Ala-His-Glu-Thr-Asn-Asn-Ser-Ala) was modeled with the DR1 molecule. The peptide was inserted with lysine inside the cleft in the hydrophilic region. This placed the Thr 5 in the center of the binding cleft and the tryptophane (residue 8) near the hydrophobic region. The resulting minimized model had ten interactions between the peptide and the protein, three interactions with the peptide backbone and five with the peptide side chains. The remaining two were with the amino terminal of the peptide. All of the interactions were in either the first three residues, His 10 or Glu 11 in the peptide. No interactions

were observed in the center of the cleft or residues four through nine.

CFA/1 with DR1:

A peptide identified as CFA/1 (colonization factor antigen) (Val-Gly-Lys-Asn-Ile-Thr-Val-Thr-Ala-Ser-Val-Asp-Pro) was prepared and an attempt was made to "fit" the molecule into the cleft of the DR1. The lysine at position 3 prevented insertion of the peptide.

Results:

The peptides chosen to dock in the DR1 model are shown in Table 1. The peptides were docked manually in several orientations into the DR1 model. The peptides were then tested in biological binding assays with the following results:

Table I

| Peptide | Molecular Model predicted binding | Binding in the bioassay |
|---|---|---|
| HA (influenza hemagglutinin) | Yes | Yes |
| HA-YK (synthetic peptide) | Yes | Yes |
| CS3 Pilin subunit | Yes | Yes |
| CFA/1 | No | No |

Quantitative measurement of the inhibition of CS3 63-78 and HA 306-318 as compared to controls is shown in Fig. 31.

The binding energy was calculated as the difference between the final DR1 and peptide complex and the sum of the energies for the minimized DR and peptide models individually. The data is shown in Table II.

Table II.

| Peptide | Protein | Residues | Sequence | Binding Energy (kcal/mol) |
|---|---|---|---|---|
| HA | Influenza hemagglutinin | 306-318 | PKYVKQNTLKLAT | -283 |
| HA-YK | synthetic peptide | | AAYAAAAAAKAA | -216 |
| CS3 | CS3 pilin subunit | 63-78 | SKNGTVTWAHETNNSA | -245 |

CS6α and CS6ß with DR1

Colonization factor antigen IV (CFA/IV is an antigen on the surface of many enterotoxigenic *E. coli* one component of which is CS6. CS6 has two major subunits and a number of minor subunits. Several peptides from CS6 have been sequenced and assayed for potential inhibition of radiolabeled HA (306-318)/DR1 complex as a measure of immunogenicity. The sequences of the subunits are shown in Table III.

Table III.

| Peptide | Amino Acid Residues | Sequence |
|---|---|---|
| CS6α6 | 63-75 | DEYGLGRLVNTAD |
| CS6α7 | 80-92 | IIYQIVDEKGKKK |
| CS6α8 | 111-123 | LNYTSGEKKISPG |
| CS6ß1 | 3-15 | WQYKSLDVNVNIE |
| CS6ß2 | 42-54 | QLYTVEMTIPAGV |
| CS6ß3 | 112-124 | TSYTFSAIYTGGE |
| CS6ß4 | 123-135 | GEYPNSGYSSGTY |
| CS6ß5 | 133-145 | GTYAGHLTVSFYS |

These peptides were assayed for inhibition of radioactively labeled HA(306-318)/DR1. The results are demonstrated in Fig. 32.

The foregoing description of the specific embodiments reveal the general nature of the invention so that others can, by applying current knowledge, readily modify and/or adapt for various applications such specific embodiments without departing from the generic concept, and, therefore, such adaptations and modifications should and are intended to be comprehended within the meaning and range of equivalents of the disclosed embodiments. It is to be understood that the phraseology or terminology employed herein is for the purpose of description and not of limitation.

All references mentioned in this application are incorporated by reference.

We Claim:

1. A method of preliminarily screening peptides for immunogenicity comprising the steps of:

1) creating a molecular model of receptor DR1 Class II MHC and minimizing the model of the DR1;

2) modeling a peptide to be tested and minimizing the model of the peptide; and

3) testing fit of model obtained in step 2 into the model obtained in step 1 to produce a composite receptor/peptide model.

2. A computerized model comprising a model of the DR1 molecule having fitted in a cleft therein a model of a peptide.

3. A method of claim 1 wherein, additionally, the receptor/peptide model is subjected to computer-simulated heating.

4. A method of claim 1 further comprising, assaying the peptide by competitive inhibition binding to a Class II MHC receptor DR1.

5. A minimized peptide capable of binding to a Class II MHC receptor DR1 and inhibiting the binding of HA (306-318).

6. A synthetic peptide, wherein the amino acid sequence of the minimized peptide according to claim 5 has been modified to have a superior binding affinity for a Class II MHC receptor DR1 to form at least a portion of the synthetic peptide.

7. A synthetic peptide, wherein the amino acid sequence of the minimized peptide according to claim 5, has been modified to have greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1 to form at least a portion of the synthetic peptide.

8. A synthetic peptide according to claim 6, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.

9. A synthetic peptide according to claim 7, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.

10. A synthetic peptide according to claim 8, wherein said uncharged amino acid is alanine.

11. A synthetic peptide according to claim 9, wherein said uncharged amino acid is alanine.

12. A minimized peptide according to claim 5, wherein the sequence is selected from the group consisting of PKYVKQNTLKLAT, AAYAAAAAAKAA and SKNGTVTWAHETNNSA.

13. A minimized peptide according to claim 5, wherein the sequence is contained in a CFA.

14. A minimized peptide according to claim 13, wherein the sequence is selected from the group consisting of DEYGLGRLVNTAD, IIYQIVDEKGKKK, LNYTSGEKKISPG, WQYKSLDVNVNIE, QLYTVEMTIPAGV, TSYTFSAIYTGGE, GEYPNSGYSSGTY and GTYAGHLTVSFYS.

15. A vaccine comprising:
a minimized peptide according to claim 5; and
an immunologically acceptable carrier.

16. A vaccine comprising:
a synthetic peptide according to claim 6; and
an immunologically acceptable carrier.

17. A vaccine comprising:
a synthetic peptide according to claim 7; and
an immunologically acceptable carrier.

18. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 15.

19. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 16.

20. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 17.

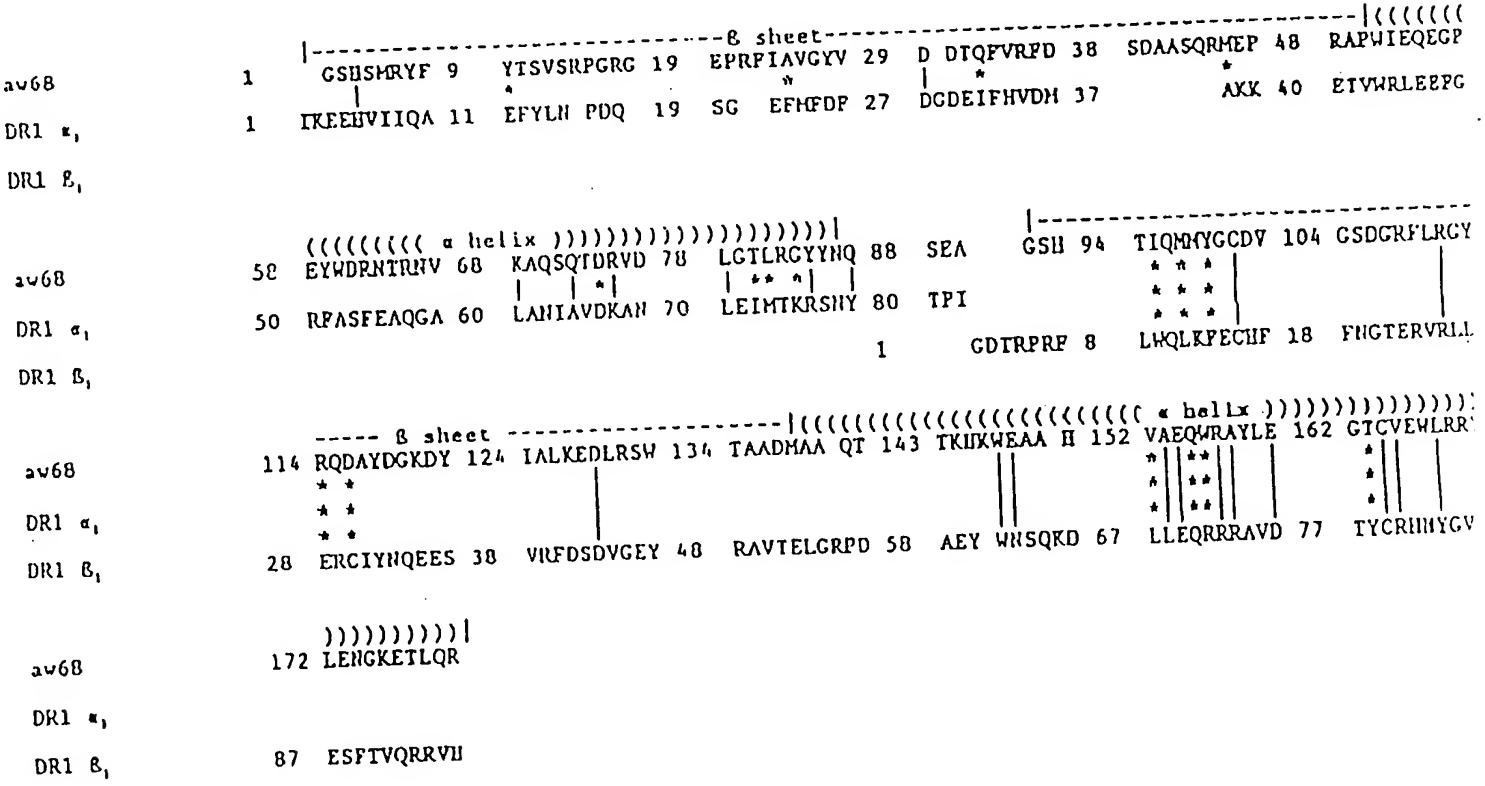
av68
DR1 α1
DR1 β1
β sheet
α helix
av68
DR1 α1
DR1 β1
av68
DR1 α1
DR1 β1
av68
DR1 α1
DR1 β1
| Conserved residues
* Polymorphic residues

FIG. 1

```
* MINIMIZED COORDINATES FROM CHARMM
*  DATE:     2/25/93     14:58:48      CREATED BY USER: naus*
*
 1839
    1     1 ILE  N     -53.41835 -52.87964  96.86949 A1    1      0.00000
    2     1 ILE  HT1   -54.06550 -53.37379  96.22549 A1    1      0.00000
    3     1 ILE  HT2   -52.48505 -53.33354  96.89426 A1    1      0.00000
    4     1 ILE  HT3   -53.81151 -52.85195  97.84341 A1    1      0.00000
    5     1 ILE  CA    -53.29159 -51.45945  96.52548 A1    1      0.00000
    6     1 ILE  CB    -54.51076 -51.09296  95.64551 A1    1      0.00000
    7     1 ILE  CG2   -55.84867 -51.39510  96.33544 A1    1      0.00000
    8     1 ILE  CG1   -54.43380 -49.65164  95.12978 A1    1      0.00000
    9     1 ILE  CD    -55.55018 -49.30658  94.14124 A1    1      0.00000
   10     1 ILE  C     -53.31306 -50.79352  97.88119 A1    1      0.00000
   11     1 ILE  O     -53.76732 -51.45486  98.80000 A1    1      0.00000
   12     2 LYS  N     -52.70566 -49.57271  97.98462 A1    2      0.00000
   13     2 LYS  H     -52.43149 -49.07042  97.19065 A1    2      0.00000
   14     2 LYS  CA    -52.72856 -48.82990  99.24363 A1    2      0.00000
   15     2 LYS  CB    -51.40674 -49.22996 100.05168 A1    2      0.00000
   16     2 LYS  CG    -51.65942 -50.46422 100.94226 A1    2      0.00000
   17     2 LYS  CD    -50.39491 -50.76541 101.74483 A1    2      0.00000
   18     2 LYS  CE    -50.65567 -51.67024 102.94896 A1    2      0.00000
   19     2 LYS  NZ    -49.48784 -51.62033 103.84066 A1    2      0.00000
   20     2 LYS  HZ1   -49.68891 -52.15413 104.71032 A1    2      0.00000
   21     2 LYS  HZ2   -48.66152 -52.03086 103.36182 A1    2      0.00000
   22     2 LYS  HZ3   -49.20787 -50.62063 104.08530 A1    2      0.00000
   23     2 LYS  C     -52.58080 -47.37619  98.05749 A1    2      0.00000
   24     2 LYS  O     -52.16561 -47.08993  97.74074 A1    2      0.00000
   25     3 GLU  N     -52.93375 -46.48610  99.78817 A1    3      0.00000
   26     3 GLU  H     -53.25920 -46.74733 100.69754 A1    3      0.00000
   27     3 GLU  CA    -52.88416 -45.05669  99.49342 A1    3      0.00000
   28     3 GLU  CB    -54.17633 -44.67728  98.75869 A1    3      0.00000
   29     3 GLU  CG    -54.16941 -43.30721  98.07127 A1    3      0.00000
   30     3 GLU  CD    -55.38365 -43.14982  97.16830 A1    3      0.00000
   31     3 GLU  OE1   -55.40070 -42.20412  96.38367 A1    3      0.00000
   32     3 GLU  OE2   -56.30088 -43.96983  97.23742 A1    3      0.00000
   33     3 GLU  C     -52.73723 -44.30588 100.80334 A1    3      0.00000
   34     3 GLU  O     -53.13310 -44.80289 101.85375 A1    3      0.00000
   35     4 GLU  N     -52.10513 -43.13147 100.72198 A1    4      0.00000
   36     4 GLU  H     -51.89913 -42.70887  99.83885 A1    4      0.00000
   37     4 GLU  CA    -51.71490 -42.41569 101.93532 A1    4      0.00000
   38     4 GLU  CB    -50.23606 -42.65775 102.23912 A1    4      0.00000
   39     4 GLU  CG    -49.88908 -44.07273 102.69972 A1    4      0.00000
   40     4 GLU  CD    -48.39447 -44.20822 102.86978 A1    4      0.00000
   41     4 GLU  OE1   -47.71593 -43.20739 103.12446 A1    4      0.00000
   42     4 GLU  OE2   -47.87485 -45.31826 102.72475 A1    4      0.00000
   43     4 GLU  C     -51.86859 -40.92476 101.75610 A1    4      0.00000
   44     4 GLU  O     -51.85445 -40.40438 100.64776 A1    4      0.00000
   45     5 HIS  N     -51.98758 -40.25490 102.89941 A1    5      0.00000
   46     5 HIS  H     -51.95529 -40.74179 103.77267 A1    5      0.00000
   47     5 HIS  CA    -52.02510 -38.79739 102.88794 A1    5      0.00000
   48     5 HIS  CB    -52.95268 -38.30654 104.00423 A1    5      0.00000
   49     5 HIS  CG    -54.39292 -38.58657 103.64511 A1    5      0.00000
   50     5 HIS  ND1   -55.01336 -38.04007 102.58831 A1    5      0.00000
   51     5 HIS  HD1   -54.63216 -37.40030 101.93314 A1    5      0.00000
   52     5 HIS  CD2   -55.29163 -39.42491 104.31043 A1    5      0.00000
   53     5 HIS  NE2   -56.46563 -39.37373 103.63249 A1    5      0.00000
   54     5 HIS  CE1   -56.29489 -38.51954 102.57197 A1    5      0.00000
   55     5 HIS  C     -50.64149 -38.20241 103.06558 A1    5      0.00000
   56     5 HIS  O     -49.75908 -38.76174 103.68940 A1    5      0.00000
   57     6 VAL  N     -50.46014 -37.02655 102.46317 A1    6      0.00000
   58     6 VAL  H     -51.22869 -36.59864 101.97707 A1    6      0.00000
   59     6 VAL  CA    -49.12695 -36.41474 102.46428 A1    6      0.00000
   60     6 VAL  CB    -48.60121 -36.33669 101.01420 A1    6      0.00000
```

FIG. 2

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 61 | 6 | VAL | CG1 | 47.07672 | -36.30119 | 101.00126 | A1 | 6 | 0.00000 |
| 62 | 6 | VAL | CG2 | 49.10544 | -37.46647 | 100.11057 | A1 | 6 | 0.00000 |
| 63 | 6 | VAL | C | -49.19435 | -35.00190 | 103.02675 | A1 | 6 | 0.00000 |
| 64 | 6 | VAL | O | -50.21018 | -34.34041 | 102.87457 | A1 | 6 | 0.00000 |
| 65 | 7 | ILE | N | -48.11527 | -34.52120 | 103.65431 | A1 | 7 | 0.00000 |
| 66 | 7 | ILE | H | -47.35972 | -35.13148 | 103.91409 | A1 | 7 | 0.00000 |
| 67 | 7 | ILE | CA | -48.09506 | -33.08697 | 103.98819 | A1 | 7 | 0.00000 |
| 68 | 7 | ILE | CB | -48.69197 | -32.86813 | 105.39701 | A1 | 7 | 0.00000 |
| 69 | 7 | ILE | CG2 | -47.96322 | -33.71317 | 106.43001 | A1 | 7 | 0.00000 |
| 70 | 7 | ILE | CG1 | -48.74316 | -31.39586 | 105.81727 | A1 | 7 | 0.00000 |
| 71 | 7 | ILE | CD | -49.28846 | -31.20489 | 107.23523 | A1 | 7 | 0.00000 |
| 72 | 7 | ILE | C | -46.69381 | -32.50114 | 103.87753 | A1 | 7 | 0.00000 |
| 73 | 7 | ILE | O | -45.72315 | -33.10109 | 104.32366 | A1 | 7 | 0.00000 |
| 74 | 8 | ILE | N | -46.61414 | -31.32789 | 103.23109 | A1 | 8 | 0.00000 |
| 75 | 8 | ILE | H | -47.43598 | -30.79777 | 103.00074 | A1 | 8 | 0.00000 |
| 76 | 8 | ILE | CA | -45.31176 | -30.85113 | 102.75879 | A1 | 8 | 0.00000 |
| 77 | 8 | ILE | CB | -45.18096 | -31.21426 | 101.24826 | A1 | 8 | 0.00000 |
| 78 | 8 | ILE | CG2 | -46.47692 | -30.98133 | 100.47371 | A1 | 8 | 0.00000 |
| 79 | 8 | ILE | CG1 | -44.01581 | -30.53590 | 100.51961 | A1 | 8 | 0.00000 |
| 80 | 8 | ILE | CD | -42.65515 | -30.85297 | 101.12422 | A1 | 8 | 0.00000 |
| 81 | 8 | ILE | C | -45.00402 | -29.37643 | 103.03239 | A1 | 8 | 0.00000 |
| 82 | 8 | ILE | O | -45.69216 | -28.43922 | 102.63903 | A1 | 8 | 0.00000 |
| 83 | 9 | GLN | N | -43.86371 | -29.19466 | 103.70229 | A1 | 9 | 0.00000 |
| 84 | 9 | GLN | H | -43.33777 | -29.97409 | 104.05676 | A1 | 9 | 0.00000 |
| 85 | 9 | GLN | CA | -43.27910 | -27.85712 | 103.71549 | A1 | 9 | 0.00000 |
| 86 | 9 | GLN | CB | -42.97213 | -27.43231 | 105.14730 | A1 | 9 | 0.00000 |
| 87 | 9 | GLN | CG | -44.24353 | -27.13894 | 105.94550 | A1 | 9 | 0.00000 |
| 88 | 9 | GLN | CD | -43.92932 | -26.69043 | 107.36359 | A1 | 9 | 0.00000 |
| 89 | 9 | GLN | OE1 | -44.59992 | -27.05224 | 108.31811 | A1 | 9 | 0.00000 |
| 90 | 9 | GLN | NE2 | -42.89278 | -25.86874 | 107.50418 | A1 | 9 | 0.00000 |
| 91 | 9 | GLN | HE21 | -42.31986 | -25.58069 | 106.73881 | A1 | 9 | 0.00000 |
| 92 | 9 | GLN | HE22 | -42.66204 | -25.53260 | 108.41526 | A1 | 9 | 0.00000 |
| 93 | 9 | GLN | C | -42.00840 | -27.79728 | 102.89330 | A1 | 9 | 0.00000 |
| 94 | 9 | GLN | O | -41.07030 | -28.56703 | 103.06902 | A1 | 9 | 0.00000 |
| 95 | 10 | ALA | N | -42.01720 | -26.84230 | 101.96835 | A1 | 10 | 0.00000 |
| 96 | 10 | ALA | H | -42.80016 | -26.24022 | 101.81084 | A1 | 10 | 0.00000 |
| 97 | 10 | ALA | CA | -40.83464 | -26.60034 | 101.15833 | A1 | 10 | 0.00000 |
| 98 | 10 | ALA | CB | -41.09424 | -26.95993 | 99.69281 | A1 | 10 | 0.00000 |
| 99 | 10 | ALA | C | -40.41733 | -25.14834 | 101.25674 | A1 | 10 | 0.00000 |
| 100 | 10 | ALA | O | -41.21138 | -24.24680 | 101.50542 | A1 | 10 | 0.00000 |
| 101 | 11 | GLU | N | -39.11637 | -24.95043 | 101.08226 | A1 | 11 | 0.00000 |
| 102 | 11 | GLU | H | -38.51800 | -25.72332 | 100.86462 | A1 | 11 | 0.00000 |
| 103 | 11 | GLU | CA | -38.56697 | -23.61077 | 101.26935 | A1 | 11 | 0.00000 |
| 104 | 11 | GLU | CB | -37.61570 | -23.62729 | 102.46404 | A1 | 11 | 0.00000 |
| 105 | 11 | GLU | CG | -38.29740 | -24.15021 | 103.73032 | A1 | 11 | 0.00000 |
| 106 | 11 | GLU | CD | -37.31724 | -24.35236 | 104.86668 | A1 | 11 | 0.00000 |
| 107 | 11 | GLU | OE1 | -37.72498 | -24.91514 | 105.87939 | A1 | 11 | 0.00000 |
| 108 | 11 | GLU | OE2 | -36.15746 | -23.95826 | 104.74301 | A1 | 11 | 0.00000 |
| 109 | 11 | GLU | C | -37.79619 | -23.17941 | 100.04756 | A1 | 11 | 0.00000 |
| 110 | 11 | GLU | O | -37.17390 | -23.99314 | 99.37097 | A1 | 11 | 0.00000 |
| 111 | 12 | PHE | N | -37.86688 | -21.87280 | 99.78525 | A1 | 12 | 0.00000 |
| 112 | 12 | PHE | H | -38.38856 | -21.25141 | 100.37827 | A1 | 12 | 0.00000 |
| 113 | 12 | PHE | CA | -37.20863 | -21.33691 | 98.59813 | A1 | 12 | 0.00000 |
| 114 | 12 | PHE | CB | -38.26225 | -21.06791 | 97.51950 | A1 | 12 | 0.00000 |
| 115 | 12 | PHE | CG | -37.93682 | -21.86124 | 96.27668 | A1 | 12 | 0.00000 |
| 116 | 12 | PHE | CD1 | -38.35291 | -23.20899 | 96.17465 | A1 | 12 | 0.00000 |
| 117 | 12 | PHE | CD2 | -37.21678 | -21.25353 | 95.22261 | A1 | 12 | 0.00000 |
| 118 | 12 | PHE | CE1 | -38.04712 | -23.95258 | 95.01356 | A1 | 12 | 0.00000 |
| 119 | 12 | PHE | CE2 | -36.91098 | -21.99741 | 94.06122 | A1 | 12 | 0.00000 |
| 120 | 12 | PHE | CZ | -37.32685 | -23.34453 | 93.96022 | A1 | 12 | 0.00000 |
| 121 | 12 | PHE | C | -36.45949 | -20.05659 | 98.90209 | A1 | 12 | 0.00000 |
| 122 | 12 | PHE | O | -37.00216 | -18.95808 | 98.93077 | A1 | 12 | 0.00000 |
| 123 | 13 | TYR | N | -35.16677 | -20.22034 | 99.15293 | A1 | 13 | 0.00000 |
| 124 | 13 | TYR | H | -34.71888 | -21.10886 | 99.03348 | A1 | 13 | 0.00000 |

FIG. 3

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 125 | 13 | TYR | CA | 4.44650 | -19.02891 | 99.57908 | A1 | 13 | 0.00000 |
| 126 | 13 | TYR | CB | -3.74164 | -19.31637 | 100.90471 | A1 | 13 | 0.00000 |
| 127 | 13 | TYR | CG | -33.63229 | -18.04844 | 101.71489 | A1 | 13 | 0.00000 |
| 128 | 13 | TYR | CD1 | -34.79192 | -17.52707 | 102.32828 | A1 | 13 | 0.00000 |
| 129 | 13 | TYR | CE1 | -34.69736 | -16.35710 | 103.10470 | A1 | 13 | 0.00000 |
| 130 | 13 | TYR | CD2 | -32.38328 | -17.40687 | 101.86606 | A1 | 13 | 0.00000 |
| 131 | 13 | TYR | CE2 | -32.29405 | -16.23332 | 102.64552 | A1 | 13 | 0.00000 |
| 132 | 13 | TYR | CZ | -33.45188 | -15.71594 | 103.26657 | A1 | 13 | 0.00000 |
| 133 | 13 | TYR | OH | -33.37191 | -14.58930 | 104.06109 | A1 | 13 | 0.00000 |
| 134 | 13 | TYR | HH | -33.47343 | -14.89238 | 104.98360 | A1 | 13 | 0.00000 |
| 135 | 13 | TYR | C | -33.46702 | -18.52544 | 98.54525 | A1 | 13 | 0.00000 |
| 136 | 13 | TYR | O | -32.59456 | -19.23915 | 98.06786 | A1 | 13 | 0.00000 |
| 137 | 14 | LEU | N | -33.65240 | -17.25550 | 98.19697 | A1 | 14 | 0.00000 |
| 138 | 14 | LEU | H | -34.33538 | -16.68306 | 98.64807 | A1 | 14 | 0.00000 |
| 139 | 14 | LEU | CA | -32.81168 | -16.70428 | 97.14258 | A1 | 14 | 0.00000 |
| 140 | 14 | LEU | CB | -33.70274 | -16.21044 | 96.00105 | A1 | 14 | 0.00000 |
| 141 | 14 | LEU | CG | -33.98219 | -17.29674 | 94.96260 | A1 | 14 | 0.00000 |
| 142 | 14 | LEU | CD1 | -35.16863 | -16.92524 | 94.07539 | A1 | 14 | 0.00000 |
| 143 | 14 | LEU | CD2 | -32.72461 | -17.54798 | 94.13078 | A1 | 14 | 0.00000 |
| 144 | 14 | LEU | C | -31.93377 | -15.56813 | 97.60481 | A1 | 14 | 0.00000 |
| 145 | 14 | LEU | O | -32.31049 | -14.71998 | 98.40126 | A1 | 14 | 0.00000 |
| 146 | 15 | ASN | N | -30.73908 | -15.58168 | 97.02166 | A1 | 15 | 0.00000 |
| 147 | 15 | ASN | H | -30.47955 | -16.38705 | 96.48149 | A1 | 15 | 0.00000 |
| 148 | 15 | ASN | CA | -29.88530 | -14.39297 | 97.02352 | A1 | 15 | 0.00000 |
| 149 | 15 | ASN | CB | -28.47094 | -14.93729 | 97.29287 | A1 | 15 | 0.00000 |
| 150 | 15 | ASN | CG | -27.86774 | -14.18957 | 98.46652 | A1 | 15 | 0.00000 |
| 151 | 15 | ASN | OD1 | -28.47231 | -13.98878 | 99.50693 | A1 | 15 | 0.00000 |
| 152 | 15 | ASN | ND2 | -26.63329 | -13.74712 | 98.26721 | A1 | 15 | 0.00000 |
| 153 | 15 | ASN | HD21 | -26.12722 | -13.93409 | 97.42633 | A1 | 15 | 0.00000 |
| 154 | 15 | ASN | HD22 | -26.21377 | -13.18778 | 98.98020 | A1 | 15 | 0.00000 |
| 155 | 15 | ASN | C | -30.09328 | -13.70870 | 95.65633 | A1 | 15 | 0.00000 |
| 156 | 15 | ASN | O | -30.96066 | -14.17939 | 94.92357 | A1 | 15 | 0.00000 |
| 157 | 16 | PRO | N | -29.35358 | -12.64312 | 95.25454 | A1 | 16 | 0.00000 |
| 158 | 16 | PRO | CD | -29.47390 | -12.14147 | 93.88390 | A1 | 16 | 0.00000 |
| 159 | 16 | PRO | CA | -28.34388 | -11.89943 | 96.02164 | A1 | 16 | 0.00000 |
| 160 | 16 | PRO | CB | -27.47317 | -11.32145 | 94.90180 | A1 | 16 | 0.00000 |
| 161 | 16 | PRO | CG | -28.40713 | -11.06430 | 93.72211 | A1 | 16 | 0.00000 |
| 162 | 16 | PRO | C | -28.87201 | -10.84560 | 96.98393 | A1 | 16 | 0.00000 |
| 163 | 16 | PRO | O | -28.49727 | -10.81095 | 98.14625 | A1 | 16 | 0.00000 |
| 164 | 17 | ASP | N | -29.73099 | -9.96981 | 96.45979 | A1 | 17 | 0.00000 |
| 165 | 17 | ASP | H | -30.06531 | -10.06794 | 95.52595 | A1 | 17 | 0.00000 |
| 166 | 17 | ASP | CA | -30.07647 | -8.75629 | 97.18869 | A1 | 17 | 0.00000 |
| 167 | 17 | ASP | CB | -30.80318 | -7.83976 | 96.20071 | A1 | 17 | 0.00000 |
| 168 | 17 | ASP | CG | -30.22601 | -6.44601 | 96.27578 | A1 | 17 | 0.00000 |
| 169 | 17 | ASP | OD1 | -29.42577 | -6.10216 | 95.40955 | A1 | 17 | 0.00000 |
| 170 | 17 | ASP | OD2 | -30.58500 | -5.71147 | 97.19272 | A1 | 17 | 0.00000 |
| 171 | 17 | ASP | C | -30.91226 | -8.96778 | 98.44177 | A1 | 17 | 0.00000 |
| 172 | 17 | ASP | O | -30.52677 | -8.65960 | 99.56331 | A1 | 17 | 0.00000 |
| 173 | 18 | GLN | N | -32.11780 | -9.49744 | 98.20428 | A1 | 18 | 0.00000 |
| 174 | 18 | GLN | H | -32.36542 | -9.81984 | 97.29256 | A1 | 18 | 0.00000 |
| 175 | 18 | GLN | CA | -33.10696 | -9.57864 | 99.27949 | A1 | 18 | 0.00000 |
| 176 | 18 | GLN | CB | -34.05728 | -8.37464 | 99.14180 | A1 | 18 | 0.00000 |
| 177 | 18 | GLN | CG | -33.36307 | -7.07517 | 99.58476 | A1 | 18 | 0.00000 |
| 178 | 18 | GLN | CD | -33.97880 | -5.85158 | 98.94046 | A1 | 18 | 0.00000 |
| 179 | 18 | GLN | OE1 | -35.13776 | -5.50918 | 99.12725 | A1 | 18 | 0.00000 |
| 180 | 18 | GLN | NE2 | -33.14378 | -5.16835 | 98.16624 | A1 | 18 | 0.00000 |
| 181 | 18 | GLN | HE21 | -32.19859 | -5.47544 | 97.99847 | A1 | 18 | 0.00000 |
| 182 | 18 | GLN | HE22 | -33.43475 | -4.32502 | 97.72302 | A1 | 18 | 0.00000 |
| 183 | 18 | GLN | C | -33.83924 | -10.91598 | 99.26964 | A1 | 18 | 0.00000 |
| 184 | 18 | GLN | O | -33.74750 | -11.68763 | 98.32391 | A1 | 18 | 0.00000 |
| 185 | 19 | SER | N | -34.51482 | -11.16924 | 100.39831 | A1 | 19 | 0.00000 |
| 186 | 19 | SER | H | -34.63228 | -10.43017 | 101.06649 | A1 | 19 | 0.00000 |
| 187 | 19 | SER | CA | -34.94474 | -12.50816 | 100.83625 | A1 | 19 | 0.00000 |
| 188 | 19 | SER | CB | -35.43672 | -12.36114 | 102.28173 | A1 | 19 | 0.00000 |

FIG. 4

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 189 | 19 | SER | OG | 34.37064 | -11.87727 | 103.10841 | A1 | 19 | 0.00000 |
| 190 | 19 | SER | HG | 33.83984 | -12.63499 | 103.40254 | A1 | 19 | 0.00000 |
| 191 | 19 | SER | C | -35.97640 | -13.29776 | 100.02197 | A1 | 19 | 0.00000 |
| 192 | 19 | SER | O | -36.49518 | -12.86400 | 99.00144 | A1 | 19 | 0.00000 |
| 193 | 20 | GLY | N | -36.24917 | -14.51787 | 100.53004 | A1 | 20 | 0.00000 |
| 194 | 20 | GLY | H | -35.87834 | -14.79673 | 101.41380 | A1 | 20 | 0.00000 |
| 195 | 20 | GLY | CA | -37.08223 | -15.47533 | 99.79192 | A1 | 20 | 0.00000 |
| 196 | 20 | GLY | C | -38.39897 | -15.89747 | 100.44590 | A1 | 20 | 0.00000 |
| 197 | 20 | GLY | O | -39.10838 | -15.10421 | 101.05171 | A1 | 20 | 0.00000 |
| 198 | 21 | GLU | N | -38.72023 | -17.18722 | 100.25477 | A1 | 21 | 0.00000 |
| 199 | 21 | GLU | H | -38.03254 | -17.84573 | 99.94375 | A1 | 21 | 0.00000 |
| 200 | 21 | GLU | CA | -40.11538 | -17.64629 | 100.27114 | A1 | 21 | 0.00000 |
| 201 | 21 | GLU | CB | -40.54163 | -17.64420 | 98.79559 | A1 | 21 | 0.00000 |
| 202 | 21 | GLU | CG | -42.00974 | -17.90322 | 98.44054 | A1 | 21 | 0.00000 |
| 203 | 21 | GLU | CD | -42.16555 | -17.98331 | 96.93169 | A1 | 21 | 0.00000 |
| 204 | 21 | GLU | OE1 | -43.22010 | -17.59671 | 96.43390 | A1 | 21 | 0.00000 |
| 205 | 21 | GLU | OE2 | -41.23758 | -18.43207 | 96.25678 | A1 | 21 | 0.00000 |
| 206 | 21 | GLU | C | -40.28326 | -19.04137 | 100.89226 | A1 | 21 | 0.00000 |
| 207 | 21 | GLU | O | -39.32286 | -19.78361 | 101.07437 | A1 | 21 | 0.00000 |
| 208 | 22 | PHE | N | -41.54286 | -19.38051 | 101.22645 | A1 | 22 | 0.00000 |
| 209 | 22 | PHE | H | -42.30204 | -18.76344 | 101.01655 | A1 | 22 | 0.00000 |
| 210 | 22 | PHE | CA | -41.84777 | -20.63223 | 101.93252 | A1 | 22 | 0.00000 |
| 211 | 22 | PHE | CB | -41.76716 | -20.31207 | 103.43794 | A1 | 22 | 0.00000 |
| 212 | 22 | PHE | CG | -41.45246 | -21.48591 | 104.34752 | A1 | 22 | 0.00000 |
| 213 | 22 | PHE | CD1 | -40.59481 | -21.25886 | 105.44915 | A1 | 22 | 0.00000 |
| 214 | 22 | PHE | CD2 | -42.01384 | -22.76966 | 104.14562 | A1 | 22 | 0.00000 |
| 215 | 22 | PHE | CE1 | -40.30109 | -22.30643 | 106.34948 | A1 | 22 | 0.00000 |
| 216 | 22 | PHE | CE2 | -41.72224 | -23.81970 | 105.04232 | A1 | 22 | 0.00000 |
| 217 | 22 | PHE | CZ | -40.86722 | -23.58408 | 106.14281 | A1 | 22 | 0.00000 |
| 218 | 22 | PHE | C | -43.25845 | -21.11988 | 101.58028 | A1 | 22 | 0.00000 |
| 219 | 22 | PHE | O | -44.19436 | -20.32985 | 101.55111 | A1 | 22 | 0.00000 |
| 220 | 23 | MET | N | -43.39639 | -22.43138 | 101.32298 | A1 | 23 | 0.00000 |
| 221 | 23 | MET | H | -42.59132 | -23.03279 | 101.30500 | A1 | 23 | 0.00000 |
| 222 | 23 | MET | CA | -44.70480 | -23.04357 | 101.02967 | A1 | 23 | 0.00000 |
| 223 | 23 | MET | CB | -45.08326 | -22.73266 | 99.57140 | A1 | 23 | 0.00000 |
| 224 | 23 | MET | CG | -46.39952 | -23.35273 | 99.09264 | A1 | 23 | 0.00000 |
| 225 | 23 | MET | SD | -46.67153 | -23.10231 | 97.33272 | A1 | 23 | 0.00000 |
| 226 | 23 | MET | CE | -47.47592 | -24.67640 | 96.98955 | A1 | 23 | 0.00000 |
| 227 | 23 | MET | C | -44.60710 | -24.56281 | 101.21411 | A1 | 23 | 0.00000 |
| 228 | 23 | MET | O | -43.70841 | -25.13566 | 100.62115 | A1 | 23 | 0.00000 |
| 229 | 24 | PHE | N | -45.43241 | -25.30285 | 101.99622 | A1 | 24 | 0.00000 |
| 230 | 24 | PHE | H | -45.17063 | -26.26850 | 102.03772 | A1 | 24 | 0.00000 |
| 231 | 24 | PHE | CA | -46.72021 | -25.11140 | 102.69060 | A1 | 24 | 0.00000 |
| 232 | 24 | PHE | CB | -47.06193 | -23.70552 | 103.21139 | A1 | 24 | 0.00000 |
| 233 | 24 | PHE | CG | -46.27878 | -23.27691 | 104.43188 | A1 | 24 | 0.00000 |
| 234 | 24 | PHE | CD1 | -46.28203 | -24.06677 | 105.60532 | A1 | 24 | 0.00000 |
| 235 | 24 | PHE | CD2 | -45.58233 | -22.04683 | 104.40480 | A1 | 24 | 0.00000 |
| 236 | 24 | PHE | CE1 | -45.58915 | -23.62279 | 106.75356 | A1 | 24 | 0.00000 |
| 237 | 24 | PHE | CE2 | -44.89083 | -21.60180 | 105.55271 | A1 | 24 | 0.00000 |
| 238 | 24 | PHE | CZ | -44.89594 | -22.39162 | 106.72434 | A1 | 24 | 0.00000 |
| 239 | 24 | PHE | C | -47.88569 | -25.61775 | 101.85776 | A1 | 24 | 0.00000 |
| 240 | 24 | PHE | O | -48.73152 | -24.87778 | 101.36424 | A1 | 24 | 0.00000 |
| 241 | 25 | ASP | N | -47.89055 | -26.94593 | 101.74049 | A1 | 25 | 0.00000 |
| 242 | 25 | ASP | H | -47.22437 | -27.52403 | 102.20704 | A1 | 25 | 0.00000 |
| 243 | 25 | ASP | CA | -48.86501 | -27.64762 | 100.90165 | A1 | 25 | 0.00000 |
| 244 | 25 | ASP | CB | -48.21052 | -27.81535 | 99.52046 | A1 | 25 | 0.00000 |
| 245 | 25 | ASP | CG | -49.19634 | -28.30012 | 98.47932 | A1 | 25 | 0.00000 |
| 246 | 25 | ASP | OD1 | -49.75750 | -27.46672 | 97.77589 | A1 | 25 | 0.00000 |
| 247 | 25 | ASP | OD2 | -49.39656 | -29.50745 | 98.38197 | A1 | 25 | 0.00000 |
| 248 | 25 | ASP | C | -49.18430 | -28.98699 | 101.56183 | A1 | 25 | 0.00000 |
| 249 | 25 | ASP | O | -48.57317 | -29.35714 | 102.56241 | A1 | 25 | 0.00000 |
| 250 | 26 | PHE | N | -50.15819 | -29.70261 | 101.00377 | A1 | 26 | 0.00000 |
| 251 | 26 | PHE | H | -50.60050 | -29.38662 | 100.15349 | A1 | 26 | 0.00000 |
| 252 | 26 | PHE | CA | -50.56030 | -30.99701 | 101.54898 | A1 | 26 | 0.00000 |

FIG. 5

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 253 | 26 | PHE | CB | 51.42378 | -30.83098 | 102.82009 | A1 | 26 | 0.00000 |
| 254 | 26 | PHE | CG | 52.60356 | -29.92038 | 102.57724 | A1 | 26 | 0.00000 |
| 255 | 26 | PHE | CD1 | -52.50398 | -28.55674 | 102.91777 | A1 | 26 | 0.00000 |
| 256 | 26 | PHE | CD2 | -53.70380 | -30.42265 | 101.99011 | A1 | 26 | 0.00000 |
| 257 | 26 | PHE | CE1 | -53.58477 | -27.68701 | 102.66706 | A1 | 26 | 0.00000 |
| 258 | 26 | PHE | CE2 | -54.86474 | -29.55076 | 101.74257 | A1 | 26 | 0.00000 |
| 259 | 26 | PHE | CZ | -54.76149 | -28.18547 | 102.07912 | A1 | 26 | 0.00000 |
| 260 | 26 | PHE | C | -51.29340 | -31.82500 | 100.51070 | A1 | 26 | 0.00000 |
| 261 | 26 | PHE | O | -51.63257 | -31.38211 | 99.42184 | A1 | 26 | 0.00000 |
| 262 | 27 | ASP | N | -51.50640 | -33.00225 | 100.89199 | A1 | 27 | 0.00000 |
| 263 | 27 | ASP | H | -51.30608 | -33.34660 | 101.83544 | A1 | 27 | 0.00000 |
| 264 | 27 | ASP | CA | -52.05815 | -34.11623 | 100.01741 | A1 | 27 | 0.00000 |
| 265 | 27 | ASP | CB | -53.56271 | -34.25359 | 100.24733 | A1 | 27 | 0.00000 |
| 266 | 27 | ASP | CG | -53.82295 | -35.66101 | 100.73899 | A1 | 27 | 0.00000 |
| 267 | 27 | ASP | OD1 | -52.95640 | -36.23164 | 101.40272 | A1 | 27 | 0.00000 |
| 268 | 27 | ASP | OD2 | -54.89062 | -36.19966 | 100.47314 | A1 | 27 | 0.00000 |
| 269 | 27 | ASP | C | -51.70102 | -34.05698 | 98.54820 | A1 | 27 | 0.00000 |
| 270 | 27 | ASP | O | -52.51335 | -34.10386 | 97.63254 | A1 | 27 | 0.00000 |
| 271 | 28 | GLY | N | -50.39045 | -33.92246 | 98.35075 | A1 | 28 | 0.00000 |
| 272 | 28 | GLY | H | -49.78144 | -33.80079 | 99.13160 | A1 | 28 | 0.00000 |
| 273 | 28 | GLY | CA | -49.88845 | -33.86633 | 96.98221 | A1 | 28 | 0.00000 |
| 274 | 28 | GLY | C | -50.00090 | -32.51821 | 96.28701 | A1 | 28 | 0.00000 |
| 275 | 28 | GLY | O | -49.04304 | -32.03342 | 95.69731 | A1 | 28 | 0.00000 |
| 276 | 29 | ASP | N | -51.21573 | -31.96145 | 96.33541 | A1 | 29 | 0.00000 |
| 277 | 29 | ASP | H | -51.93955 | -32.39453 | 96.87595 | A1 | 29 | 0.00000 |
| 278 | 29 | ASP | CA | -51.52130 | -30.85124 | 95.43198 | A1 | 29 | 0.00000 |
| 279 | 29 | ASP | CB | -52.38232 | -31.44665 | 94.30287 | A1 | 29 | 0.00000 |
| 280 | 29 | ASP | CG | -52.46245 | -30.54960 | 93.07981 | A1 | 29 | 0.00000 |
| 281 | 29 | ASP | OD1 | -51.43429 | -30.32445 | 92.44162 | A1 | 29 | 0.00000 |
| 282 | 29 | ASP | OD2 | -53.56233 | -30.10545 | 92.75048 | A1 | 29 | 0.00000 |
| 283 | 29 | ASP | C | -52.21461 | -29.64631 | 96.07233 | A1 | 29 | 0.00000 |
| 284 | 29 | ASP | O | -52.39419 | -28.59407 | 95.46732 | A1 | 29 | 0.00000 |
| 285 | 30 | GLU | N | -52.65130 | -29.81701 | 97.32405 | A1 | 30 | 0.00000 |
| 286 | 30 | GLU | H | -52.34793 | -30.57647 | 97.90251 | A1 | 30 | 0.00000 |
| 287 | 30 | GLU | CA | -53.43516 | -28.70871 | 97.86160 | A1 | 30 | 0.00000 |
| 288 | 30 | GLU | CB | -54.71008 | -29.18152 | 98.54724 | A1 | 30 | 0.00000 |
| 289 | 30 | GLU | CG | -55.84100 | -29.71506 | 97.67444 | A1 | 30 | 0.00000 |
| 290 | 30 | GLU | CD | -57.13279 | -29.50058 | 98.43828 | A1 | 30 | 0.00000 |
| 291 | 30 | GLU | OE1 | -57.79466 | -30.47326 | 98.78969 | A1 | 30 | 0.00000 |
| 292 | 30 | GLU | OE2 | -57.48939 | -28.34297 | 98.66447 | A1 | 30 | 0.00000 |
| 293 | 30 | GLU | C | -52.69655 | -27.80995 | 98.82987 | A1 | 30 | 0.00000 |
| 294 | 30 | GLU | O | -52.13191 | -28.20198 | 99.84476 | A1 | 30 | 0.00000 |
| 295 | 31 | ILE | N | -52.76110 | -26.53268 | 98.46810 | A1 | 31 | 0.00000 |
| 296 | 31 | ILE | H | -53.28532 | -26.29454 | 97.65353 | A1 | 31 | 0.00000 |
| 297 | 31 | ILE | CA | -51.98442 | -25.52556 | 99.18511 | A1 | 31 | 0.00000 |
| 298 | 31 | ILE | CB | -51.81933 | -24.32331 | 98.23317 | A1 | 31 | 0.00000 |
| 299 | 31 | ILE | CG2 | -53.16329 | -23.65625 | 97.91607 | A1 | 31 | 0.00000 |
| 300 | 31 | ILE | CG1 | -50.75168 | -23.33810 | 98.71478 | A1 | 31 | 0.00000 |
| 301 | 31 | ILE | CD | -50.41981 | -22.27940 | 97.66271 | A1 | 31 | 0.00000 |
| 302 | 31 | ILE | C | -52.51316 | -25.12446 | 100.56211 | A1 | 31 | 0.00000 |
| 303 | 31 | ILE | O | -53.70233 | -24.97567 | 100.82175 | A1 | 31 | 0.00000 |
| 304 | 32 | PHE | N | -51.54696 | -24.95576 | 101.46562 | A1 | 32 | 0.00000 |
| 305 | 32 | PHE | H | -50.59061 | -25.06998 | 101.18020 | A1 | 32 | 0.00000 |
| 306 | 32 | PHE | CA | -51.85606 | -24.57978 | 102.84494 | A1 | 32 | 0.00000 |
| 307 | 32 | PHE | CB | -50.76201 | -25.18703 | 103.73391 | A1 | 32 | 0.00000 |
| 308 | 32 | PHE | CG | -51.19588 | -26.22218 | 104.74893 | A1 | 32 | 0.00000 |
| 309 | 32 | PHE | CD1 | -50.23927 | -27.18148 | 105.15120 | A1 | 32 | 0.00000 |
| 310 | 32 | PHE | CD2 | -52.49149 | -26.22907 | 105.32111 | A1 | 32 | 0.00000 |
| 311 | 32 | PHE | CE1 | -50.57386 | -28.14516 | 106.12524 | A1 | 32 | 0.00000 |
| 312 | 32 | PHE | CE2 | -52.82688 | -27.19600 | 106.29575 | A1 | 32 | 0.00000 |
| 313 | 32 | PHE | CZ | -51.86606 | -28.15152 | 106.69566 | A1 | 32 | 0.00000 |
| 314 | 32 | PHE | C | -51.84397 | -23.07181 | 103.07985 | A1 | 32 | 0.00000 |
| 315 | 32 | PHE | O | -52.76581 | -22.46086 | 103.62205 | A1 | 32 | 0.00000 |
| 316 | 33 | HIS | N | -50.69098 | -22.50451 | 102.70813 | A1 | 33 | 0.00000 |

FIG. 6

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 317 | 33 | HIS | H | 0.04312 | -22.98834 | 102.10786 | A1 | 33 | 0.00000 |
| 318 | 33 | HIS | CA | -50.22576 | -21.21727 | 103.23242 | A1 | 33 | 0.00000 |
| 319 | 33 | HIS | CB | -49.65908 | -21.51540 | 104.63303 | A1 | 33 | 0.00000 |
| 320 | 33 | HIS | CG | -49.22984 | -20.32142 | 105.45366 | A1 | 33 | 0.00000 |
| 321 | 33 | HIS | ND1 | -48.02826 | -19.72793 | 105.37205 | A1 | 33 | 0.00000 |
| 322 | 33 | HIS | HD1 | -47.28999 | -19.92757 | 104.75923 | A1 | 33 | 0.00000 |
| 323 | 33 | HIS | CD2 | -49.97214 | -19.68828 | 106.45019 | A1 | 33 | 0.00000 |
| 324 | 33 | HIS | NE2 | -49.20118 | -18.70682 | 106.97086 | A1 | 33 | 0.00000 |
| 325 | 33 | HIS | CE1 | -48.00110 | -18.72654 | 106.30763 | A1 | 33 | 0.00000 |
| 326 | 33 | HIS | C | -49.11511 | -20.78472 | 102.29629 | A1 | 33 | 0.00000 |
| 327 | 33 | HIS | O | -48.59725 | -21.61206 | 101.55845 | A1 | 33 | 0.00000 |
| 328 | 34 | VAL | N | -48.74537 | -19.50449 | 102.33695 | A1 | 34 | 0.00000 |
| 329 | 34 | VAL | H | -49.19429 | -18.80802 | 102.90183 | A1 | 34 | 0.00000 |
| 330 | 34 | VAL | CA | -47.51776 | -19.11490 | 101.64269 | A1 | 34 | 0.00000 |
| 331 | 34 | VAL | CB | -47.81303 | -18.42567 | 100.28392 | A1 | 34 | 0.00000 |
| 332 | 34 | VAL | CG1 | -46.56686 | -18.41158 | 99.39158 | A1 | 34 | 0.00000 |
| 333 | 34 | VAL | CG2 | -48.95871 | -19.06363 | 99.49806 | A1 | 34 | 0.00000 |
| 334 | 34 | VAL | C | -46.79652 | -18.14692 | 102.56509 | A1 | 34 | 0.00000 |
| 335 | 34 | VAL | O | -47.41849 | -17.54298 | 103.42874 | A1 | 34 | 0.00000 |
| 336 | 35 | ASP | N--- | -45.47963 | -18.03426 | 102.37666 | A1 | 35 | 0.00000 |
| 337 | 35 | ASP | H | -45.03039 | -18.68906 | 101.76710 | A1 | 35 | 0.00000 |
| 338 | 35 | ASP | CA | -44.68799 | -16.93300 | 102.93355 | A1 | 35 | 0.00000 |
| 339 | 35 | ASP | CB | -44.74876 | -15.73492 | 101.94639 | A1 | 35 | 0.00000 |
| 340 | 35 | ASP | CG | -46.11850 | -15.06364 | 101.88569 | A1 | 35 | 0.00000 |
| 341 | 35 | ASP | OD1 | -46.85196 | -15.31279 | 100.93528 | A1 | 35 | 0.00000 |
| 342 | 35 | ASP | OD2 | -46.43780 | -14.28565 | 102.78747 | A1 | 35 | 0.00000 |
| 343 | 35 | ASP | C | -44.90949 | -16.57120 | 104.41152 | A1 | 35 | 0.00000 |
| 344 | 35 | ASP | O | -45.03304 | -17.43137 | 105.27733 | A1 | 35 | 0.00000 |
| 345 | 36 | MET | N | -44.91212 | -15.26386 | 104.68945 | A1 | 36 | 0.00000 |
| 346 | 36 | MET | H | -44.97503 | -14.58792 | 103.95356 | A1 | 36 | 0.00000 |
| 347 | 36 | MET | CA | -45.05621 | -14.74244 | 106.04065 | A1 | 36 | 0.00000 |
| 348 | 36 | MET | CB | -44.58443 | -13.28473 | 106.01845 | A1 | 36 | 0.00000 |
| 349 | 36 | MET | CG | -43.15122 | -13.10955 | 105.50403 | A1 | 36 | 0.00000 |
| 350 | 36 | MET | SD | -42.96722 | -11.71848 | 104.37016 | A1 | 36 | 0.00000 |
| 351 | 36 | MET | CE | -43.60204 | -10.40582 | 105.42531 | A1 | 36 | 0.00000 |
| 352 | 36 | MET | C | -46.49207 | -14.77022 | 106.53712 | A1 | 36 | 0.00000 |
| 353 | 36 | MET | O | -46.75425 | -14.73983 | 107.73458 | A1 | 36 | 0.00000 |
| 354 | 37 | ALA | N | -47.43476 | -14.78996 | 105.58618 | A1 | 37 | 0.00000 |
| 355 | 37 | ALA | H | -47.21869 | -14.87225 | 104.60519 | A1 | 37 | 0.00000 |
| 356 | 37 | ALA | CA | -48.80100 | -14.57493 | 106.05297 | A1 | 37 | 0.00000 |
| 357 | 37 | ALA | CB | -49.30059 | -13.19637 | 105.61316 | A1 | 37 | 0.00000 |
| 358 | 37 | ALA | C | -49.83252 | -15.61256 | 105.65673 | A1 | 37 | 0.00000 |
| 359 | 37 | ALA | O | -49.85254 | -16.18787 | 104.57639 | A1 | 37 | 0.00000 |
| 360 | 38 | LYS | N | -50.76933 | -15.79391 | 106.59397 | A1 | 38 | 0.00000 |
| 361 | 38 | LYS | H | -50.65212 | -15.37866 | 107.49351 | A1 | 38 | 0.00000 |
| 362 | 38 | LYS | CA | -52.00981 | -16.48765 | 106.23832 | A1 | 38 | 0.00000 |
| 363 | 38 | LYS | CB | -52.90628 | -16.55867 | 107.48308 | A1 | 38 | 0.00000 |
| 364 | 38 | LYS | CG | -52.41585 | -17.40517 | 108.60236 | A1 | 38 | 0.00000 |
| 365 | 38 | LYS | CD | -53.40991 | -18.62084 | 108.86903 | A1 | 38 | 0.00000 |
| 366 | 38 | LYS | CE | -53.42547 | -19.66155 | 107.75111 | A1 | 38 | 0.00000 |
| 367 | 38 | LYS | NZ | -54.78503 | -20.17861 | 107.56038 | A1 | 38 | 0.00000 |
| 368 | 38 | LYS | HZ1 | -54.79226 | -20.92377 | 106.83759 | A1 | 38 | 0.00000 |
| 369 | 38 | LYS | HZ2 | -55.17879 | -20.59510 | 108.44046 | A1 | 38 | 0.00000 |
| 370 | 38 | LYS | HZ3 | -55.42747 | -19.41621 | 107.27224 | A1 | 38 | 0.00000 |
| 371 | 38 | LYS | C | -52.74081 | -15.73437 | 105.12989 | A1 | 38 | 0.00000 |
| 372 | 38 | LYS | O | -52.72521 | -14.51209 | 105.10297 | A1 | 38 | 0.00000 |
| 373 | 39 | LYS | N | -53.35457 | -16.44351 | 104.17702 | A1 | 39 | 0.00000 |
| 374 | 39 | LYS | H | -53.59774 | -15.96113 | 103.33578 | A1 | 39 | 0.00000 |
| 375 | 39 | LYS | CA | -53.67982 | -17.86931 | 104.22041 | A1 | 39 | 0.00000 |
| 376 | 39 | LYS | CB | -55.18971 | -18.00506 | 104.55346 | A1 | 39 | 0.00000 |
| 377 | 39 | LYS | CG | -56.24681 | -17.84030 | 103.42417 | A1 | 39 | 0.00000 |
| 378 | 39 | LYS | CD | -56.27039 | -16.52580 | 102.62130 | A1 | 39 | 0.00000 |
| 379 | 39 | LYS | CE | -56.64532 | -16.69161 | 101.13213 | A1 | 39 | 0.00000 |
| 380 | 39 | LYS | NZ | -55.66137 | -17.54082 | 100.43802 | A1 | 39 | 0.00000 |

FIG. 7

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 381 | 39 | LYS | HZ1 | 55.95645 | -18.54581 | 100.36313 | A1 | 3 | 0.00000 |
| 382 | 39 | LYS | HZ2 | -55.39863 | -17.26725 | 99.46103 | A1 | 39 | 0.00000 |
| 383 | 39 | LYS | HZ3 | -54.72486 | -17.51921 | 100.90690 | A1 | 39 | 0.00000 |
| 384 | 39 | LYS | C | -53.44423 | -18.44283 | 102.84433 | A1 | 39 | 0.00000 |
| 385 | 39 | LYS | O | -53.43351 | -17.67518 | 101.88936 | A1 | 39 | 0.00000 |
| 386 | 40 | GLU | N | -53.41332 | -19.77420 | 102.71885 | A1 | 40 | 0.00000 |
| 387 | 40 | GLU | H | -53.16154 | -20.43691 | 103.42697 | A1 | 40 | 0.00000 |
| 388 | 40 | GLU | CA | -54.08892 | -20.14645 | 101.48663 | A1 | 40 | 0.00000 |
| 389 | 40 | GLU | CB | -53.22132 | -20.84643 | 100.44056 | A1 | 40 | 0.00000 |
| 390 | 40 | GLU | CG | -52.68203 | -19.82757 | 99.41114 | A1 | 40 | 0.00000 |
| 391 | 40 | GLU | CD | -53.78227 | -18.90107 | 98.89631 | A1 | 40 | 0.00000 |
| 392 | 40 | GLU | OE1 | -53.60681 | -17.68372 | 98.89245 | A1 | 40 | 0.00000 |
| 393 | 40 | GLU | OE2 | -54.88246 | -19.35560 | 98.59153 | A1 | 40 | 0.00000 |
| 394 | 40 | GLU | C | -55.46625 | -20.74566 | 101.61501 | A1 | 40 | 0.00000 |
| 395 | 40 | GLU | O | -56.42031 | -20.18304 | 101.08479 | A1 | 40 | 0.00000 |
| 396 | 41 | THR | N | -55.56321 | -21.84976 | 102.35754 | A1 | 41 | 0.00000 |
| 397 | 41 | THR | H | -54.77319 | -22.20472 | 102.86321 | A1 | 41 | 0.00000 |
| 398 | 41 | THR | CA | -56.84476 | -22.55464 | 102.30963 | A1 | 41 | 0.00000 |
| 399 | 41 | THR | CB | -56.55011 | -24.05030 | 102.16109 | A1 | 41 | 0.00000 |
| 400 | 41 | THR | OG1 | -57.73042 | -24.75407 | 101.74066 | A1 | 41 | 0.00000 |
| 401 | 41 | THR | HG1 | -57.47835 | -25.59614 | 101.33840 | A1 | 41 | 0.00000 |
| 402 | 41 | THR | CG2 | -55.95304 | -24.67173 | 103.43152 | A1 | 41 | 0.00000 |
| 403 | 41 | THR | C | -57.85722 | -22.26510 | 103.42344 | A1 | 41 | 0.00000 |
| 404 | 41 | THR | O | -57.54877 | -21.93546 | 104.56718 | A1 | 41 | 0.00000 |
| 405 | 42 | VAL | N | -59.12316 | -22.41525 | 103.00455 | A1 | 42 | 0.00000 |
| 406 | 42 | VAL | H | -59.25687 | -22.81422 | 102.09633 | A1 | 42 | 0.00000 |
| 407 | 42 | VAL | CA | -60.29134 | -22.03291 | 103.80812 | A1 | 42 | 0.00000 |
| 408 | 42 | VAL | CB | -61.57611 | -22.26846 | 102.98525 | A1 | 42 | 0.00000 |
| 409 | 42 | VAL | CG1 | -62.83989 | -21.83994 | 103.74041 | A1 | 42 | 0.00000 |
| 410 | 42 | VAL | CG2 | -61.49852 | -21.55078 | 101.63610 | A1 | 42 | 0.00000 |
| 411 | 42 | VAL | C | -60.39368 | -22.75550 | 105.14170 | A1 | 42 | 0.00000 |
| 412 | 42 | VAL | O | -60.54018 | -22.16641 | 106.20404 | A1 | 42 | 0.00000 |
| 413 | 43 | TRP | N | -60.26652 | -24.07997 | 105.07466 | A1 | 43 | 0.00000 |
| 414 | 43 | TRP | H | -60.09540 | -24.53437 | 104.20145 | A1 | 43 | 0.00000 |
| 415 | 43 | TRP | CA | -60.35178 | -24.82113 | 106.34002 | A1 | 43 | 0.00000 |
| 416 | 43 | TRP | CB | -60.91225 | -26.25321 | 106.17013 | A1 | 43 | 0.00000 |
| 417 | 43 | TRP | CG | -60.96314 | -26.72686 | 104.73262 | A1 | 43 | 0.00000 |
| 418 | 43 | TRP | CD2 | -59.88712 | -27.12198 | 103.92127 | A1 | 43 | 0.00000 |
| 419 | 43 | TRP | CE2 | -60.47947 | -27.49629 | 102.60102 | A1 | 43 | 0.00000 |
| 420 | 43 | TRP | CE3 | -58.50029 | -27.24274 | 104.12574 | A1 | 43 | 0.00000 |
| 421 | 43 | TRP | CD1 | -62.11826 | -26.86040 | 103.93459 | A1 | 43 | 0.00000 |
| 422 | 43 | TRP | NE1 | -61.84174 | -27.31306 | 102.67766 | A1 | 43 | 0.00000 |
| 423 | 43 | TRP | HE1 | -62.50030 | -27.49046 | 101.97106 | A1 | 43 | 0.00000 |
| 424 | 43 | TRP | CZ2 | -59.62565 | -27.96652 | 101.58525 | A1 | 43 | 0.00000 |
| 425 | 43 | TRP | CZ3 | -57.69263 | -27.72260 | 103.07694 | A1 | 43 | 0.00000 |
| 426 | 43 | TRP | CH2 | -58.24204 | -28.07937 | 101.82597 | A1 | 43 | 0.00000 |
| 427 | 43 | TRP | C | -59.07150 | -24.84373 | 107.16564 | A1 | 43 | 0.00000 |
| 428 | 43 | TRP | O | -58.85050 | -25.68073 | 108.02836 | A1 | 43 | 0.00000 |
| 429 | 44 | ARG | N | -58.22471 | -23.84563 | 106.89519 | A1 | 44 | 0.00000 |
| 430 | 44 | ARG | H | -58.31398 | -23.27977 | 106.07364 | A1 | 44 | 0.00000 |
| 431 | 44 | ARG | CA | -57.22046 | -23.49560 | 107.89144 | A1 | 44 | 0.00000 |
| 432 | 44 | ARG | CB | -55.83244 | -23.69727 | 107.26013 | A1 | 44 | 0.00000 |
| 433 | 44 | ARG | CG | -54.63741 | -23.63473 | 108.22026 | A1 | 44 | 0.00000 |
| 434 | 44 | ARG | CD | -53.30915 | -23.64273 | 107.47006 | A1 | 44 | 0.00000 |
| 435 | 44 | ARG | NE | -52.18625 | -23.26000 | 108.32672 | A1 | 44 | 0.00000 |
| 436 | 44 | ARG | HE | -52.36221 | -22.91543 | 109.25139 | A1 | 44 | 0.00000 |
| 437 | 44 | ARG | CZ | -50.93149 | -23.33650 | 107.86475 | A1 | 44 | 0.00000 |
| 438 | 44 | ARG | NH1 | -49.92358 | -22.86519 | 108.56844 | A1 | 44 | 0.00000 |
| 439 | 44 | ARG | HH11 | -48.98076 | -22.84912 | 108.24673 | A1 | 44 | 0.00000 |
| 440 | 44 | ARG | HH12 | -50.05162 | -22.52238 | 109.51721 | A1 | 44 | 0.00000 |
| 441 | 44 | ARG | NH2 | -50.67215 | -23.89024 | 106.69352 | A1 | 44 | 0.00000 |
| 442 | 44 | ARG | HH21 | -49.73581 | -23.96008 | 106.35139 | A1 | 44 | 0.00000 |
| 443 | 44 | ARG | HH22 | -51.41769 | -24.25918 | 106.14195 | A1 | 44 | 0.00000 |
| 444 | 44 | ARG | C | -57.42751 | -22.05857 | 108.38029 | A1 | 44 | 0.00000 |

FIG. 8

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 445 | 44 | ARG | O | 6.53064 | -21.39201 | 108.88943 | A1 | 44 | 0.00000 |
| 446 | 45 | LEU | N | -58.65270 | -21.55686 | 108.18548 | A1 | 45 | 0.00000 |
| 447 | 45 | LEU | H | -59.36846 | -22.06382 | 107.69729 | A1 | 45 | 0.00000 |
| 448 | 45 | LEU | CA | -58.94679 | -20.21897 | 108.70611 | A1 | 45 | 0.00000 |
| 449 | 45 | LEU | CB | -59.87267 | -19.46515 | 107.74942 | A1 | 45 | 0.00000 |
| 450 | 45 | LEU | CG | -59.15056 | -18.96990 | 106.49579 | A1 | 45 | 0.00000 |
| 451 | 45 | LEU | CD1 | -60.14534 | -18.41906 | 105.47407 | A1 | 45 | 0.00000 |
| 452 | 45 | LEU | CD2 | -58.10431 | -17.92289 | 106.87944 | A1 | 45 | 0.00000 |
| 453 | 45 | LEU | C | -59.55818 | -20.20104 | 110.09168 | A1 | 45 | 0.00000 |
| 454 | 45 | LEU | O | -59.53362 | -19.19926 | 110.79199 | A1 | 45 | 0.00000 |
| 455 | 46 | GLU | N | -60.08917 | -21.36024 | 110.48954 | A1 | 46 | 0.00000 |
| 456 | 46 | GLU | H | -60.14047 | -22.14708 | 109.87631 | A1 | 46 | 0.00000 |
| 457 | 46 | GLU | CA | -60.58379 | -21.47317 | 111.86481 | A1 | 46 | 0.00000 |
| 458 | 46 | GLU | CB | -61.47817 | -22.71518 | 111.95437 | A1 | 46 | 0.00000 |
| 459 | 46 | GLU | CG | -60.80881 | -24.02385 | 111.51772 | A1 | 46 | 0.00000 |
| 460 | 46 | GLU | CD | -61.85264 | -25.11830 | 111.46594 | A1 | 46 | 0.00000 |
| 461 | 46 | GLU | OE1 | -62.26867 | -25.47222 | 110.36424 | A1 | 46 | 0.00000 |
| 462 | 46 | GLU | OE2 | -62.24894 | -25.60616 | 112.52280 | A1 | 46 | 0.00000 |
| 463 | 46 | GLU | C | -59.48698 | -21.49323 | 112.92683 | A1 | 46 | 0.00000 |
| 464 | 46 | GLU | O | -59.60959 | -21.22226 | 114.10493 | A1 | 46 | 0.00000 |
| 465 | 47 | GLU | N | -58.27888 | -21.79310 | 112.44220 | A1 | 47 | 0.00000 |
| 466 | 47 | GLU | H | -58.18142 | -22.06659 | 111.48920 | A1 | 47 | 0.00000 |
| 467 | 47 | GLU | CA | -57.08155 | -21.73864 | 113.27698 | A1 | 47 | 0.00000 |
| 468 | 47 | GLU | CB | -55.89121 | -22.09481 | 112.39059 | A1 | 47 | 0.00000 |
| 469 | 47 | GLU | CG | -55.95036 | -23.50661 | 111.78977 | A1 | 47 | 0.00000 |
| 470 | 47 | GLU | CD | -55.55418 | -24.58648 | 112.78701 | A1 | 47 | 0.00000 |
| 471 | 47 | GLU | OE1 | -55.48886 | -25.74409 | 112.37878 | A1 | 47 | 0.00000 |
| 472 | 47 | GLU | OE2 | -55.29749 | -24.27876 | 113.95212 | A1 | 47 | 0.00000 |
| 473 | 47 | GLU | C | -56.83827 | -20.38151 | 113.91510 | A1 | 47 | 0.00000 |
| 474 | 47 | GLU | O | -56.67000 | -19.35742 | 113.26194 | A1 | 47 | 0.00000 |
| 475 | 48 | PHE | N | -56.83807 | -20.40716 | 115.24713 | A1 | 48 | 0.00000 |
| 476 | 48 | PHE | H | -56.92233 | -21.28123 | 115.72305 | A1 | 48 | 0.00000 |
| 477 | 48 | PHE | CA | -56.75617 | -19.13647 | 115.96362 | A1 | 48 | 0.00000 |
| 478 | 48 | PHE | CB | -57.20231 | -19.34982 | 117.41420 | A1 | 48 | 0.00000 |
| 479 | 48 | PHE | CG | -58.41697 | -18.49841 | 117.70829 | A1 | 48 | 0.00000 |
| 480 | 48 | PHE | CD1 | -59.71122 | -19.00320 | 117.44215 | A1 | 48 | 0.00000 |
| 481 | 48 | PHE | CD2 | -58.25459 | -17.19966 | 118.24455 | A1 | 48 | 0.00000 |
| 482 | 48 | PHE | CE1 | -60.84630 | -18.20670 | 117.71246 | A1 | 48 | 0.00000 |
| 483 | 48 | PHE | CE2 | -59.38940 | -16.40286 | 118.51469 | A1 | 48 | 0.00000 |
| 484 | 48 | PHE | CZ | -60.68202 | -16.90878 | 118.24779 | A1 | 48 | 0.00000 |
| 485 | 48 | PHE | C | -55.39240 | -18.46628 | 115.93777 | A1 | 48 | 0.00000 |
| 486 | 48 | PHE | O | -54.35117 | -19.07618 | 115.72587 | A1 | 48 | 0.00000 |
| 487 | 49 | GLY | N | -55.43214 | -17.15361 | 116.19781 | A1 | 49 | 0.00000 |
| 488 | 49 | GLY | H | -56.32069 | -16.72101 | 116.34575 | A1 | 49 | 0.00000 |
| 489 | 49 | GLY | CA | -54.23420 | -16.30520 | 116.13162 | A1 | 49 | 0.00000 |
| 490 | 49 | GLY | C | -52.92695 | -16.86464 | 116.68056 | A1 | 49 | 0.00000 |
| 491 | 49 | GLY | O | -51.85815 | -16.69886 | 116.10714 | A1 | 49 | 0.00000 |
| 492 | 50 | ARG | N | -53.03915 | -17.56211 | 117.81779 | A1 | 50 | 0.00000 |
| 493 | 50 | ARG | H | -53.93666 | -17.67284 | 118.24069 | A1 | 50 | 0.00000 |
| 494 | 50 | ARG | CA | -51.84656 | -18.16800 | 118.42224 | A1 | 50 | 0.00000 |
| 495 | 50 | ARG | CB | -52.27437 | -18.92760 | 119.68340 | A1 | 50 | 0.00000 |
| 496 | 50 | ARG | CG | -51.10260 | -19.32736 | 120.58254 | A1 | 50 | 0.00000 |
| 497 | 50 | ARG | CD | -51.53002 | -20.14774 | 121.80047 | A1 | 50 | 0.00000 |
| 498 | 50 | ARG | NE | -50.37432 | -20.44943 | 122.64580 | A1 | 50 | 0.00000 |
| 499 | 50 | ARG | HE | -49.69865 | -19.71957 | 122.75767 | A1 | 50 | 0.00000 |
| 500 | 50 | ARG | CZ | -50.24449 | -21.63184 | 123.26571 | A1 | 50 | 0.00000 |
| 501 | 50 | ARG | NH1 | -49.18578 | -21.84466 | 124.04503 | A1 | 50 | 0.00000 |
| 502 | 50 | ARG | HH11 | -49.05579 | -22.71179 | 124.52612 | A1 | 50 | 0.00000 |
| 503 | 50 | ARG | HH12 | -48.49360 | -21.13233 | 124.16453 | A1 | 50 | 0.00000 |
| 504 | 50 | ARG | NH2 | -51.15926 | -22.58829 | 123.10823 | A1 | 50 | 0.00000 |
| 505 | 50 | ARG | HH21 | -51.08073 | -23.47414 | 123.56513 | A1 | 50 | 0.00000 |
| 506 | 50 | ARG | HH22 | -51.95092 | -22.42795 | 122.51852 | A1 | 50 | 0.00000 |
| 507 | 50 | ARG | C | -51.06703 | -19.09581 | 117.49074 | A1 | 50 | 0.00000 |
| 508 | 50 | ARG | O | -49.84240 | -19.09133 | 117.41926 | A1 | 50 | 0.00000 |

FIG. 9

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 509 | 51 | PHE | N | -51.84915 | -19.87778 | 116.73839 | A1 | 51 | 0.00000 |
| 510 | 51 | PHE | H | -52.84564 | -19.76657 | 116.76797 | A1 | 51 | 0.00000 |
| 511 | 51 | PHE | CA | -51.29477 | -20.78796 | 115.73402 | A1 | 51 | 0.00000 |
| 512 | 51 | PHE | CB | -52.51672 | -21.52503 | 115.15449 | A1 | 51 | 0.00000 |
| 513 | 51 | PHE | CG | -52.25099 | -22.49194 | 114.02359 | A1 | 51 | 0.00000 |
| 514 | 51 | PHE | CD1 | -51.87888 | -23.82851 | 114.29503 | A1 | 51 | 0.00000 |
| 515 | 51 | PHE | CD2 | -52.45788 | -22.06484 | 112.69289 | A1 | 51 | 0.00000 |
| 516 | 51 | PHE | CE1 | -51.72483 | -24.74421 | 113.22969 | A1 | 51 | 0.00000 |
| 517 | 51 | PHE | CE2 | -52.30778 | -22.98082 | 111.63059 | A1 | 51 | 0.00000 |
| 518 | 51 | PHE | CZ | -51.94314 | -24.31860 | 111.90000 | A1 | 51 | 0.00000 |
| 519 | 51 | PHE | C | -50.50268 | -20.00696 | 114.69371 | A1 | 51 | 0.00000 |
| 520 | 51 | PHE | O | -49.31281 | -20.20801 | 114.47961 | A1 | 51 | 0.00000 |
| 521 | 52 | ALA | N | -51.20469 | -19.03212 | 114.10202 | A1 | 52 | 0.00000 |
| 522 | 52 | ALA | H | -52.16823 | -18.89764 | 114.33870 | A1 | 52 | 0.00000 |
| 523 | 52 | ALA | CA | -50.54896 | -18.16486 | 113.11957 | A1 | 52 | 0.00000 |
| 524 | 52 | ALA | CB | -51.52058 | -17.09216 | 112.62511 | A1 | 52 | 0.00000 |
| 525 | 52 | ALA | C | -49.28257 | -17.48933 | 113.62687 | A1 | 52 | 0.00000 |
| 526 | 52 | ALA | O | -48.27008 | -17.39834 | 112.94510 | A1 | 52 | 0.00000 |
| 527 | 53 | SER | N | -49.35763 | -17.04955 | 114.88764 | A1 | 53 | 0.00000 |
| 528 | 53 | SER | H | -50.22411 | -17.11498 | 115.38567 | A1 | 53 | 0.00000 |
| 529 | 53 | SER | CA | -48.18100 | -16.47055 | 115.53815 | A1 | 53 | 0.00000 |
| 530 | 53 | SER | CB | -48.58146 | -16.02158 | 116.95383 | A1 | 53 | 0.00000 |
| 531 | 53 | SER | OG | -47.59593 | -15.15541 | 117.52845 | A1 | 53 | 0.00000 |
| 532 | 53 | SER | HG | -47.05158 | -14.90357 | 118.42105 | A1 | 53 | 0.00000 |
| 533 | 53 | SER | C | -46.99433 | -17.42737 | 115.57426 | A1 | 53 | 0.00000 |
| 534 | 53 | SER | O | -45.89463 | -17.11790 | 115.12568 | A1 | 53 | 0.00000 |
| 535 | 54 | PHE | N | -47.26082 | -18.64220 | 116.08200 | A1 | 54 | 0.00000 |
| 536 | 54 | PHE | H | -48.18040 | -18.87361 | 116.41568 | A1 | 54 | 0.00000 |
| 537 | 54 | PHE | CA | -46.18727 | -19.64350 | 116.09999 | A1 | 54 | 0.00000 |
| 538 | 54 | PHE | CB | -46.69548 | -20.99079 | 116.63413 | A1 | 54 | 0.00000 |
| 539 | 54 | PHE | CG | -46.90625 | -20.99411 | 118.13255 | A1 | 54 | 0.00000 |
| 540 | 54 | PHE | CD1 | -48.11656 | -21.50316 | 118.65539 | A1 | 54 | 0.00000 |
| 541 | 54 | PHE | CD2 | -45.89246 | -20.53119 | 119.00621 | A1 | 54 | 0.00000 |
| 542 | 54 | PHE | CE1 | -48.31310 | -21.55376 | 120.05266 | A1 | 54 | 0.00000 |
| 543 | 54 | PHE | CE2 | -46.08993 | -20.57973 | 120.40382 | A1 | 54 | 0.00000 |
| 544 | 54 | PHE | CZ | -47.30008 | -21.09192 | 120.92307 | A1 | 54 | 0.00000 |
| 545 | 54 | PHE | C | -45.57270 | -19.90650 | 114.73758 | A1 | 54 | 0.00000 |
| 546 | 54 | PHE | O | -44.36030 | -19.93109 | 114.55246 | A1 | 54 | 0.00000 |
| 547 | 55 | GLU | N | -46.46681 | -20.08976 | 113.76558 | A1 | 55 | 0.00000 |
| 548 | 55 | GLU | H | -47.45338 | -20.04226 | 113.95516 | A1 | 55 | 0.00000 |
| 549 | 55 | GLU | CA | -45.97322 | -20.41545 | 112.42886 | A1 | 55 | 0.00000 |
| 550 | 55 | GLU | CB | -47.14512 | -20.81915 | 111.54876 | A1 | 55 | 0.00000 |
| 551 | 55 | GLU | CG | -47.92567 | -21.96126 | 112.19274 | A1 | 55 | 0.00000 |
| 552 | 55 | GLU | CD | -49.04456 | -22.36202 | 111.27677 | A1 | 55 | 0.00000 |
| 553 | 55 | GLU | OE1 | -49.15553 | -23.53977 | 110.96047 | A1 | 55 | 0.00000 |
| 554 | 55 | GLU | OE2 | -49.80524 | -21.50984 | 110.81474 | A1 | 55 | 0.00000 |
| 555 | 55 | GLU | C | -45.19354 | -19.30188 | 111.76318 | A1 | 55 | 0.00000 |
| 556 | 55 | GLU | O | -44.12678 | -19.50387 | 111.19343 | A1 | 55 | 0.00000 |
| 557 | 56 | ALA | N | -45.73650 | -18.08673 | 111.89532 | A1 | 56 | 0.00000 |
| 558 | 56 | ALA | H | -46.62336 | -17.96765 | 112.34890 | A1 | 56 | 0.00000 |
| 559 | 56 | ALA | CA | -45.00414 | -16.92733 | 111.38640 | A1 | 56 | 0.00000 |
| 560 | 56 | ALA | CB | -45.80074 | -15.63871 | 111.59969 | A1 | 56 | 0.00000 |
| 561 | 56 | ALA | C | -43.63772 | -16.77849 | 112.02791 | A1 | 56 | 0.00000 |
| 562 | 56 | ALA | O | -42.62065 | -16.60634 | 111.36878 | A1 | 56 | 0.00000 |
| 563 | 57 | GLN | N | -43.63088 | -16.91454 | 113.35929 | A1 | 57 | 0.00000 |
| 564 | 57 | GLN | H | -44.48826 | -17.03983 | 113.86832 | A1 | 57 | 0.00000 |
| 565 | 57 | GLN | CA | -42.35063 | -16.88200 | 114.06847 | A1 | 57 | 0.00000 |
| 566 | 57 | GLN | CB | -42.61987 | -17.03049 | 115.56930 | A1 | 57 | 0.00000 |
| 567 | 57 | GLN | CG | -41.40659 | -16.75355 | 116.45895 | A1 | 57 | 0.00000 |
| 568 | 57 | GLN | CD | -41.80070 | -16.94589 | 117.90800 | A1 | 57 | 0.00000 |
| 569 | 57 | GLN | OE1 | -42.29879 | -16.06206 | 118.58910 | A1 | 57 | 0.00000 |
| 570 | 57 | GLN | NE2 | -41.55425 | -18.16011 | 118.38366 | A1 | 57 | 0.00000 |
| 571 | 57 | GLN | HE21 | -41.14709 | -18.87176 | 117.81428 | A1 | 57 | 0.00000 |
| 572 | 57 | GLN | HE22 | -41.78115 | -18.36728 | 119.33313 | A1 | 57 | 0.00000 |

FIG. 10

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 573 | 57 | GLN | C | 1.36213 | -17.94055 | 113.59025 | A1 | 57 | 0.00000 |
| 574 | 57 | GLN | O | -40.18971 | -17.68051 | 113.34773 | A1 | 57 | 0.00000 |
| 575 | 58 | GLY | N | -41.88825 | -19.15742 | 113.41319 | A1 | 58 | 0.00000 |
| 576 | 58 | GLY | H | -42.84771 | -19.33514 | 113.64847 | A1 | 58 | 0.00000 |
| 577 | 58 | GLY | CA | -41.05379 | -20.23393 | 112.87374 | A1 | 58 | 0.00000 |
| 578 | 58 | GLY | C | -40.45534 | -19.92701 | 111.50957 | A1 | 58 | 0.00000 |
| 579 | 58 | GLY | O | -39.25324 | -20.01021 | 111.27849 | A1 | 58 | 0.00000 |
| 580 | 59 | ALA | N | -41.34654 | -19.52227 | 110.60018 | A1 | 59 | 0.00000 |
| 581 | 59 | ALA | H | -42.32072 | -19.46762 | 110.83485 | A1 | 59 | 0.00000 |
| 582 | 59 | ALA | CA | -40.88666 | -19.14537 | 109.26181 | A1 | 59 | 0.00000 |
| 583 | 59 | ALA | CB | -42.07124 | -18.74086 | 108.30101 | A1 | 59 | 0.00000 |
| 584 | 59 | ALA | C | -39.86090 | -18.02257 | 109.26073 | A1 | 59 | 0.00000 |
| 585 | 59 | ALA | O | -38.85187 | -18.04905 | 108.56603 | A1 | 59 | 0.00000 |
| 586 | 60 | LEU | N | -40.12979 | -17.02925 | 110.11113 | A1 | 60 | 0.00000 |
| 587 | 60 | LEU | H | -40.96678 | -17.03715 | 110.66448 | A1 | 60 | 0.00000 |
| 588 | 60 | LEU | CA | -39.17026 | -15.93079 | 110.21454 | A1 | 60 | 0.00000 |
| 589 | 60 | LEU | CB | -39.82974 | -14.72108 | 110.88234 | A1 | 60 | 0.00000 |
| 590 | 60 | LEU | CG | -41.00342 | -14.16448 | 110.06267 | A1 | 60 | 0.00000 |
| 591 | 60 | LEU | CD1 | -41.72077 | -13.05637 | 110.83175 | A1 | 60 | 0.00000 |
| 592 | 60 | LEU | CD2 | -40.54968 | -13.69403 | 108.67852 | A1 | 60 | 0.00000 |
| 593 | 60 | LEU | C | -37.86300 | -16.28607 | 110.90549 | A1 | 60 | 0.00000 |
| 594 | 60 | LEU | O | -36.81366 | -15.71151 | 110.64266 | A1 | 60 | 0.00000 |
| 595 | 61 | ALA | N | -37.92548 | -17.30628 | 111.76650 | A1 | 61 | 0.00000 |
| 596 | 61 | ALA | H | -38.80416 | -17.70206 | 112.04737 | A1 | 61 | 0.00000 |
| 597 | 61 | ALA | CA | -36.66060 | -17.86080 | 112.25036 | A1 | 61 | 0.00000 |
| 598 | 61 | ALA | CB | -36.90091 | -18.87147 | 113.37402 | A1 | 61 | 0.00000 |
| 599 | 61 | ALA | C | -35.86652 | -18.52303 | 111.13575 | A1 | 61 | 0.00000 |
| 600 | 61 | ALA | O | -34.67753 | -18.28483 | 110.93578 | A1 | 61 | 0.00000 |
| 601 | 62 | ASN | N | -36.59182 | -19.33811 | 110.35468 | A1 | 62 | 0.00000 |
| 602 | 62 | ASN | H | -37.55651 | -19.52444 | 110.56458 | A1 | 62 | 0.00000 |
| 603 | 62 | ASN | CA | -35.93048 | -19.97053 | 109.20954 | A1 | 62 | 0.00000 |
| 604 | 62 | ASN | CB | -36.90608 | -20.83397 | 108.41185 | A1 | 62 | 0.00000 |
| 605 | 62 | ASN | CG | -36.14296 | -21.97501 | 107.76767 | A1 | 62 | 0.00000 |
| 606 | 62 | ASN | OD1 | -35.90083 | -23.00051 | 108.38915 | A1 | 62 | 0.00000 |
| 607 | 62 | ASN | ND2 | -35.81296 | -21.80385 | 106.49294 | A1 | 62 | 0.00000 |
| 608 | 62 | ASN | HD21 | -35.71613 | -20.90910 | 106.04169 | A1 | 62 | 0.00000 |
| 609 | 62 | ASN | HD22 | -35.64736 | -22.62041 | 105.92778 | A1 | 62 | 0.00000 |
| 610 | 62 | ASN | C | -35.27272 | -18.97317 | 108.27635 | A1 | 62 | 0.00000 |
| 611 | 62 | ASN | O | -34.08977 | -19.05772 | 107.98073 | A1 | 62 | 0.00000 |
| 612 | 63 | ILE | N | -36.07385 | -17.96130 | 107.91224 | A1 | 63 | 0.00000 |
| 613 | 63 | ILE | H | -37.03805 | -17.97906 | 108.18770 | A1 | 63 | 0.00000 |
| 614 | 63 | ILE | CA | -35.60960 | -16.86395 | 107.05550 | A1 | 63 | 0.00000 |
| 615 | 63 | ILE | CB | -36.79680 | -15.88630 | 106.84927 | A1 | 63 | 0.00000 |
| 616 | 63 | ILE | CG2 | -36.71800 | -14.58751 | 107.66300 | A1 | 63 | 0.00000 |
| 617 | 63 | ILE | CG1 | -37.00443 | -15.60068 | 105.36486 | A1 | 63 | 0.00000 |
| 618 | 63 | ILE | CD | -36.27181 | -14.79756 | 105.06416 | A1 | 63 | 0.00000 |
| 619 | 63 | ILE | C | -34.32421 | -16.14412 | 107.48562 | A1 | 63 | 0.00000 |
| 620 | 63 | ILE | O | -33.67028 | -15.43835 | 106.72047 | A1 | 63 | 0.00000 |
| 621 | 64 | ALA | N | -33.97867 | -16.34078 | 108.76481 | A1 | 64 | 0.00000 |
| 622 | 64 | ALA | H | -34.55914 | -16.88095 | 109.37800 | A1 | 64 | 0.00000 |
| 623 | 64 | ALA | CA | -32.68252 | -15.86370 | 109.23001 | A1 | 64 | 0.00000 |
| 624 | 64 | ALA | CB | -32.78414 | -15.37252 | 110.67448 | A1 | 64 | 0.00000 |
| 625 | 64 | ALA | C | -31.59324 | -16.91956 | 109.13883 | A1 | 64 | 0.00000 |
| 626 | 64 | ALA | O | -30.45701 | -16.65389 | 108.75412 | A1 | 64 | 0.00000 |
| 627 | 65 | VAL | N | -31.96250 | -18.15367 | 109.50633 | A1 | 65 | 0.00000 |
| 628 | 65 | VAL | H | -32.92093 | -18.37377 | 109.71401 | A1 | 65 | 0.00000 |
| 629 | 65 | VAL | CA | -30.91507 | -19.17596 | 109.47932 | A1 | 65 | 0.00000 |
| 630 | 65 | VAL | CB | -31.28412 | -20.41152 | 110.33210 | A1 | 65 | 0.00000 |
| 631 | 65 | VAL | CG1 | -31.53866 | -19.97521 | 111.77524 | A1 | 65 | 0.00000 |
| 632 | 65 | VAL | CG2 | -32.45603 | -21.23819 | 109.79675 | A1 | 65 | 0.00000 |
| 633 | 65 | VAL | C | -30.45713 | -19.56758 | 108.08237 | A1 | 65 | 0.00000 |
| 634 | 65 | VAL | O | -29.26868 | -19.71596 | 107.82437 | A1 | 65 | 0.00000 |
| 635 | 66 | ASP | N | -31.42136 | -19.66037 | 107.15805 | A1 | 66 | 0.00000 |
| 636 | 66 | ASP | H | -32.38553 | -19.49723 | 107.38832 | A1 | 66 | 0.00000 |

FIG. 11

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 637 | 66 | ASP | CA | -31.04858 | -19.93216 | 105.76795 | A1 | 66 | 0.00000 |
| 638 | 66 | ASP | CB | -32.31036 | -20.24966 | 104.93007 | A1 | 66 | 0.00000 |
| 639 | 66 | ASP | CG | -33.44297 | -19.24219 | 105.08208 | A1 | 66 | 0.00000 |
| 640 | 66 | ASP | OD1 | -33.16986 | -18.05114 | 105.20729 | A1 | 66 | 0.00000 |
| 641 | 66 | ASP | OD2 | -34.60286 | -19.65468 | 105.08126 | A1 | 66 | 0.00000 |
| 642 | 66 | ASP | C | -30.18178 | -18.83449 | 105.15564 | A1 | 66 | 0.00000 |
| 643 | 66 | ASP | O | -29.16482 | -19.06872 | 104.50705 | A1 | 66 | 0.00000 |
| 644 | 67 | LYS | N | -30.56424 | -17.59916 | 105.48017 | A1 | 67 | 0.00000 |
| 645 | 67 | LYS | H | -31.49538 | -17.48655 | 105.84055 | A1 | 67 | 0.00000 |
| 646 | 67 | LYS | CA | -29.72959 | -16.43204 | 105.19320 | A1 | 67 | 0.00000 |
| 647 | 67 | LYS | CB | -30.39071 | -15.23196 | 105.87104 | A1 | 67 | 0.00000 |
| 648 | 67 | LYS | CG | -29.79159 | -13.86177 | 105.56853 | A1 | 67 | 0.00000 |
| 649 | 67 | LYS | CD | -30.51506 | -12.79056 | 106.38164 | A1 | 67 | 0.00000 |
| 650 | 67 | LYS | CE | -29.96446 | -11.38645 | 106.14720 | A1 | 67 | 0.00000 |
| 651 | 67 | LYS | NZ | -30.68526 | -10.44891 | 107.01869 | A1 | 67 | 0.00000 |
| 652 | 67 | LYS | HZ1 | -30.33262 | -9.48398 | 106.85909 | A1 | 67 | 0.00000 |
| 653 | 67 | LYS | HZ2 | -31.70143 | -10.49161 | 106.80064 | A1 | 67 | 0.00000 |
| 654 | 67 | LYS | HZ3 | -30.53221 | -10.71804 | 108.01156 | A1 | 67 | 0.00000 |
| 655 | 67 | LYS | C | -28.28117 | -16.58093 | 105.64383 | A1 | 67 | 0.00000 |
| 656 | 67 | LYS | O | -27.33559 | -16.44078 | 104.87661 | A1 | 67 | 0.00000 |
| 657 | 68 | ALA | N | -28.12520 | -16.92373 | 106.92795 | A1 | 68 | 0.00000 |
| 658 | 68 | ALA | H | -28.92119 | -17.00935 | 107.53692 | A1 | 68 | 0.00000 |
| 659 | 68 | ALA | CA | -26.76352 | -17.18143 | 107.40958 | A1 | 68 | 0.00000 |
| 660 | 68 | ALA | CB | -26.77377 | -17.44846 | 108.91534 | A1 | 68 | 0.00000 |
| 661 | 68 | ALA | C | -26.07149 | -18.34364 | 106.70618 | A1 | 68 | 0.00000 |
| 662 | 68 | ALA | O | -24.80989 | -18.33297 | 106.37143 | A1 | 68 | 0.00000 |
| 663 | 69 | ASN | N | -26.87877 | -19.37475 | 106.44973 | A1 | 69 | 0.00000 |
| 664 | 69 | ASN | H | -27.84416 | -19.34421 | 106.72158 | A1 | 69 | 0.00000 |
| 665 | 69 | ASN | CA | -26.32826 | -20.54731 | 105.77098 | A1 | 69 | 0.00000 |
| 666 | 69 | ASN | CB | -27.33794 | -21.70567 | 105.74618 | A1 | 69 | 0.00000 |
| 667 | 69 | ASN | CG | -27.75534 | -22.20215 | 107.12937 | A1 | 69 | 0.00000 |
| 668 | 69 | ASN | OD1 | -28.81753 | -22.77967 | 107.30600 | A1 | 69 | 0.00000 |
| 669 | 69 | ASN | ND2 | -26.90880 | -21.98927 | 108.13718 | A1 | 69 | 0.00000 |
| 670 | 69 | ASN | HD21 | -26.02949 | -21.53117 | 108.03476 | A1 | 69 | 0.00000 |
| 671 | 69 | ASN | HD22 | -27.17968 | -22.29754 | 109.04652 | A1 | 69 | 0.00000 |
| 672 | 69 | ASN | C | -25.83413 | -20.26827 | 104.36379 | A1 | 69 | 0.00000 |
| 673 | 69 | ASN | O | -24.88019 | -20.87816 | 103.89106 | A1 | 69 | 0.00000 |
| 674 | 70 | LEU | N | -26.46696 | -19.27268 | 103.71664 | A1 | 70 | 0.00000 |
| 675 | 70 | LEU | H | -27.27121 | -18.83110 | 104.12686 | A1 | 70 | 0.00000 |
| 676 | 70 | LEU | CA | -25.93555 | -18.80513 | 102.42930 | A1 | 70 | 0.00000 |
| 677 | 70 | LEU | CB | -26.70466 | -17.57714 | 101.93156 | A1 | 70 | 0.00000 |
| 678 | 70 | LEU | CG | -28.07464 | -17.87907 | 101.32608 | A1 | 70 | 0.00000 |
| 679 | 70 | LEU | CD1 | -28.90878 | -16.60756 | 101.23109 | A1 | 70 | 0.00000 |
| 680 | 70 | LEU | CD2 | -27.93286 | -18.56192 | 99.96378 | A1 | 70 | 0.00000 |
| 681 | 70 | LEU | C | -24.47328 | -18.42736 | 102.51389 | A1 | 70 | 0.00000 |
| 682 | 70 | LEU | O | -23.64160 | -18.86456 | 101.72791 | A1 | 70 | 0.00000 |
| 683 | 71 | GLU | N | -24.17065 | -17.62592 | 103.54240 | A1 | 71 | 0.00000 |
| 684 | 71 | GLU | H | -24.87529 | -17.33320 | 104.19342 | A1 | 71 | 0.00000 |
| 685 | 71 | GLU | CA | -22.77384 | -17.24207 | 103.73624 | A1 | 71 | 0.00000 |
| 686 | 71 | GLU | CB | -22.68099 | -16.23884 | 104.88750 | A1 | 71 | 0.00000 |
| 687 | 71 | GLU | CG | -21.33647 | -15.50613 | 104.93364 | A1 | 71 | 0.00000 |
| 688 | 71 | GLU | CD | -21.30052 | -14.53829 | 106.10023 | A1 | 71 | 0.00000 |
| 689 | 71 | GLU | OE1 | -20.27115 | -14.47665 | 106.76970 | A1 | 71 | 0.00000 |
| 690 | 71 | GLU | OE2 | -22.29376 | -13.85012 | 106.33423 | A1 | 71 | 0.00000 |
| 691 | 71 | GLU | C | -21.86369 | -18.43808 | 103.97868 | A1 | 71 | 0.00000 |
| 692 | 71 | GLU | O | -20.81243 | -18.61050 | 103.36820 | A1 | 71 | 0.00000 |
| 693 | 72 | ILE | N | -22.34609 | -19.31836 | 104.86364 | A1 | 72 | 0.00000 |
| 694 | 72 | ILE | H | -23.21301 | -19.12129 | 105.33200 | A1 | 72 | 0.00000 |
| 695 | 72 | ILE | CA | -21.56703 | -20.53142 | 105.13649 | A1 | 72 | 0.00000 |
| 696 | 72 | ILE | CB | -22.29516 | -21.40405 | 106.17923 | A1 | 72 | 0.00000 |
| 697 | 72 | ILE | CG2 | -21.51796 | -22.68646 | 106.50604 | A1 | 72 | 0.00000 |
| 698 | 72 | ILE | CG1 | -22.55172 | -20.59465 | 107.45409 | A1 | 72 | 0.00000 |
| 699 | 72 | ILE | CD | -23.34520 | -21.36378 | 108.51180 | A1 | 72 | 0.00000 |
| 700 | 72 | ILE | C | -21.22106 | -21.35113 | 103.89490 | A1 | 72 | 0.00000 |

FIG. 12

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 701 | 72 | ILE | O | 20.06679 | -21.68162 | 103.64178 | A1 | 72 | 0.00000 |
| 702 | 73 | MET | N | -22.24406 | -21.67127 | 103.09738 | A1 | 73 | 0.00000 |
| 703 | 73 | MET | H | -23.17806 | -21.34412 | 103.27303 | A1 | 73 | 0.00000 |
| 704 | 73 | MET | CA | -21.88577 | -22.51146 | 101.95532 | A1 | 73 | 0.00000 |
| 705 | 73 | MET | CB | -23.02917 | -23.44601 | 101.56487 | A1 | 73 | 0.00000 |
| 706 | 73 | MET | CG | -23.30745 | -24.44882 | 102.69030 | A1 | 73 | 0.00000 |
| 707 | 73 | MET | SD | -24.39480 | -25.79652 | 102.19686 | A1 | 73 | 0.00000 |
| 708 | 73 | MET | CE | -24.58745 | -26.56731 | 103.81212 | A1 | 73 | 0.00000 |
| 709 | 73 | MET | C | -21.30840 | -21.79430 | 100.75010 | A1 | 73 | 0.00000 |
| 710 | 73 | MET | O | -20.54740 | -22.36938 | 99.97894 | A1 | 73 | 0.00000 |
| 711 | 74 | THR | N | -21.60342 | -20.49214 | 100.63510 | A1 | 74 | 0.00000 |
| 712 | 74 | THR | H | -22.28955 | -20.04403 | 101.21510 | A1 | 74 | 0.00000 |
| 713 | 74 | THR | CA | -20.82593 | -19.73833 | 99.64704 | A1 | 74 | 0.00000 |
| 714 | 74 | THR | CB | -21.46299 | -18.35496 | 99.36040 | A1 | 74 | 0.00000 |
| 715 | 74 | THR | OG1 | -21.01301 | -17.84761 | 98.09669 | A1 | 74 | 0.00000 |
| 716 | 74 | THR | HG1 | -20.04699 | -17.88381 | 98.02785 | A1 | 74 | 0.00000 |
| 717 | 74 | THR | CG2 | -21.20740 | -17.31089 | 100.44667 | A1 | 74 | 0.00000 |
| 718 | 74 | THR | C | -19.35170 | -19.61359 | 100.02467 | A1 | 74 | 0.00000 |
| 719 | 74 | THR | O | -18.48554 | -19.49348 | 99.16750 | A1 | 74 | 0.00000 |
| 720 | 75 | LYS | N | -19.08538 | -19.69260 | 101.33717 | A1 | 75 | 0.00000 |
| 721 | 75 | LYS | H | -19.81875 | -19.65220 | 102.02321 | A1 | 75 | 0.00000 |
| 722 | 75 | LYS | CA | -17.69833 | -19.83955 | 101.77078 | A1 | 75 | 0.00000 |
| 723 | 75 | LYS | CB | -17.61408 | -19.57287 | 103.27797 | A1 | 75 | 0.00000 |
| 724 | 75 | LYS | CG | -16.20208 | -19.66153 | 103.86107 | A1 | 75 | 0.00000 |
| 725 | 75 | LYS | CD | -16.21091 | -19.57437 | 105.38567 | A1 | 75 | 0.00000 |
| 726 | 75 | LYS | CE | -14.81504 | -19.74395 | 105.98417 | A1 | 75 | 0.00000 |
| 727 | 75 | LYS | NZ | -14.91179 | -19.69891 | 107.44939 | A1 | 75 | 0.00000 |
| 728 | 75 | LYS | HZ1 | -13.96820 | -19.83508 | 107.86470 | A1 | 75 | 0.00000 |
| 729 | 75 | LYS | HZ2 | -15.29159 | -18.77551 | 107.74094 | A1 | 75 | 0.00000 |
| 730 | 75 | LYS | HZ3 | -15.54844 | -20.45311 | 107.77639 | A1 | 75 | 0.00000 |
| 731 | 75 | LYS | C | -17.14118 | -21.21778 | 101.45102 | A1 | 75 | 0.00000 |
| 732 | 75 | LYS | O | -16.11623 | -21.36022 | 100.79660 | A1 | 75 | 0.00000 |
| 733 | 76 | ARG | N | -17.86151 | -22.25466 | 101.90990 | A1 | 76 | 0.00000 |
| 734 | 76 | ARG | H | -18.69512 | -22.09296 | 102.44436 | A1 | 76 | 0.00000 |
| 735 | 76 | ARG | CA | -17.35520 | -23.61422 | 101.67525 | A1 | 76 | 0.00000 |
| 736 | 76 | ARG | CB | -18.33654 | -24.68494 | 102.17145 | A1 | 76 | 0.00000 |
| 737 | 76 | ARG | CG | -18.82789 | -24.66219 | 103.62361 | A1 | 76 | 0.00000 |
| 738 | 76 | ARG | CD | -19.55383 | -25.98411 | 103.91795 | A1 | 76 | 0.00000 |
| 739 | 76 | ARG | NE | -20.36155 | -25.99642 | 105.14334 | A1 | 76 | 0.00000 |
| 740 | 76 | ARG | HE | -21.34527 | -25.85364 | 105.02467 | A1 | 76 | 0.00000 |
| 741 | 76 | ARG | CZ | -19.85069 | -26.28686 | 106.34915 | A1 | 76 | 0.00000 |
| 742 | 76 | ARG | NH1 | -20.67426 | -26.45770 | 107.38550 | A1 | 76 | 0.00000 |
| 743 | 76 | ARG | HH11 | -20.32038 | -26.64144 | 108.30551 | A1 | 76 | 0.00000 |
| 744 | 76 | ARG | HH12 | -21.67206 | -26.42100 | 107.26619 | A1 | 76 | 0.00000 |
| 745 | 76 | ARG | NH2 | -18.53304 | -26.41209 | 106.51158 | A1 | 76 | 0.00000 |
| 746 | 76 | ARG | HH21 | -18.12377 | -26.62371 | 107.39854 | A1 | 76 | 0.00000 |
| 747 | 76 | ARG | HH22 | -17.92942 | -26.29542 | 105.72237 | A1 | 76 | 0.00000 |
| 748 | 76 | ARG | C | -17.06072 | -23.91761 | 100.20901 | A1 | 76 | 0.00000 |
| 749 | 76 | ARG | O | -16.02715 | -24.45819 | 99.83552 | A1 | 76 | 0.00000 |
| 750 | 77 | SER | N | -18.01091 | -23.50462 | 99.36716 | A1 | 77 | 0.00000 |
| 751 | 77 | SER | H | -18.84286 | -23.05363 | 99.69917 | A1 | 77 | 0.00000 |
| 752 | 77 | SER | CA | -17.80506 | -23.71642 | 97.93702 | A1 | 77 | 0.00000 |
| 753 | 77 | SER | CB | -19.13837 | -24.15898 | 97.32351 | A1 | 77 | 0.00000 |
| 754 | 77 | SER | OG | -18.92403 | -25.08061 | 96.24728 | A1 | 77 | 0.00000 |
| 755 | 77 | SER | HG | -18.99574 | -24.62840 | 95.39572 | A1 | 77 | 0.00000 |
| 756 | 77 | SER | C | -17.22854 | -22.51234 | 97.20137 | A1 | 77 | 0.00000 |
| 757 | 77 | SER | O | -17.39865 | -22.33993 | 96.00106 | A1 | 77 | 0.00000 |
| 758 | 78 | ASN | N | -16.52714 | -21.66944 | 97.97646 | A1 | 78 | 0.00000 |
| 759 | 78 | ASN | H | -16.44843 | -21.84082 | 98.96113 | A1 | 78 | 0.00000 |
| 760 | 78 | ASN | CA | -15.74721 | -20.53857 | 97.45264 | A1 | 78 | 0.00000 |
| 761 | 78 | ASN | CB | -14.33390 | -21.01377 | 97.09195 | A1 | 78 | 0.00000 |
| 762 | 78 | ASN | CG | -13.52905 | -21.21984 | 98.36114 | A1 | 78 | 0.00000 |
| 763 | 78 | ASN | OD1 | -12.89966 | -20.31632 | 98.89264 | A1 | 78 | 0.00000 |
| 764 | 78 | ASN | ND2 | -13.55264 | -22.45457 | 98.85326 | A1 | 78 | 0.00000 |

FIG. 13

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 765 | 78 | ASN | HD21 | 4.08412 | -23.19170 | 98.43678 | A1 | 78 | 0.00000 |
| 766 | 78 | ASN | HD22 | -13.03871 | -22.65362 | 99.68493 | A1 | 78 | 0.00000 |
| 767 | 78 | ASN | C | -16.34134 | -19.72172 | 96.31352 | A1 | 78 | 0.00000 |
| 768 | 78 | ASN | O | -15.71478 | -19.42979 | 95.30178 | A1 | 78 | 0.00000 |
| 769 | 79 | TYR | N | -17.59612 | -19.32597 | 96.52354 | A1 | 79 | 0.00000 |
| 770 | 79 | TYR | H | -18.05424 | -19.55771 | 97.38252 | A1 | 79 | 0.00000 |
| 771 | 79 | TYR | CA | -18.21408 | -18.48918 | 95.49858 | A1 | 79 | 0.00000 |
| 772 | 79 | TYR | CB | -19.64874 | -18.92649 | 95.21260 | A1 | 79 | 0.00000 |
| 773 | 79 | TYR | CG | -19.74485 | -20.32764 | 94.65360 | A1 | 79 | 0.00000 |
| 774 | 79 | TYR | CD1 | -20.64246 | -21.23278 | 95.25950 | A1 | 79 | 0.00000 |
| 775 | 79 | TYR | CE1 | -20.76017 | -22.54189 | 94.75217 | A1 | 79 | 0.00000 |
| 776 | 79 | TYR | CD2 | -18.96361 | -20.72112 | 93.54108 | A1 | 79 | 0.00000 |
| 777 | 79 | TYR | CE2 | -19.07884 | -22.03339 | 93.03642 | A1 | 79 | 0.00000 |
| 778 | 79 | TYR | CZ | -19.97533 | -22.93822 | 93.64752 | A1 | 79 | 0.00000 |
| 779 | 79 | TYR | OH | -20.07585 | -24.23438 | 93.18578 | A1 | 79 | 0.00000 |
| 780 | 79 | TYR | HH | -19.67682 | -24.30670 | 92.31232 | A1 | 79 | 0.00000 |
| 781 | 79 | TYR | C | -18.21035 | -17.01261 | 95.83719 | A1 | 79 | 0.00000 |
| 782 | 79 | TYR | O | -18.85099 | -16.51273 | 96.76683 | A1 | 79 | 0.00000 |
| 783 | 80 | THR | N | -17.42457 | -16.33235 | 95.00452 | A1 | 80 | 0.00000 |
| 784 | 80 | THR | H | -16.96429 | -16.79509 | 94.24288 | A1 | 80 | 0.00000 |
| 785 | 80 | THR | CA | -17.09577 | -14.92660 | 95.20513 | A1 | 80 | 0.00000 |
| 786 | 80 | THR | CB | -15.89072 | -14.87711 | 96.18098 | A1 | 80 | 0.00000 |
| 787 | 80 | THR | OG1 | -15.49849 | -13.52440 | 96.43537 | A1 | 80 | 0.00000 |
| 788 | 80 | THR | HG1 | -14.60960 | -13.50159 | 96.80560 | A1 | 80 | 0.00000 |
| 789 | 80 | THR | CG2 | -14.69719 | -15.72265 | 95.72104 | A1 | 80 | 0.00000 |
| 790 | 80 | THR | C | -16.77512 | -14.32258 | 93.83840 | A1 | 80 | 0.00000 |
| 791 | 80 | THR | O | -16.16879 | -14.97644 | 92.99811 | A1 | 80 | 0.00000 |
| 792 | 81 | PRO | N | -17.23243 | -13.08096 | 93.61451 | A1 | 81 | 0.00000 |
| 793 | 81 | PRO | CD | -18.04687 | -12.25452 | 94.50529 | A1 | 81 | 0.00000 |
| 794 | 81 | PRO | CA | -16.95963 | -12.43774 | 92.32255 | A1 | 81 | 0.00000 |
| 795 | 81 | PRO | CB | -18.08102 | -11.39225 | 92.28996 | A1 | 81 | 0.00000 |
| 796 | 81 | PRO | CG | -18.22970 | -10.94901 | 93.74456 | A1 | 81 | 0.00000 |
| 797 | 81 | PRO | C | -15.57247 | -11.80328 | 92.25040 | A1 | 81 | 0.00000 |
| 798 | 81 | PRO | O | -15.41926 | -10.58936 | 92.16776 | A1 | 81 | 0.00000 |
| 799 | 82 | ILE | N | -14.55883 | -12.66988 | 92.27154 | A1 | 82 | 0.00000 |
| 800 | 82 | ILE | H | -14.69364 | -13.66392 | 92.31920 | A1 | 82 | 0.00000 |
| 801 | 82 | ILE | CA | -13.18946 | -12.18130 | 92.13921 | A1 | 82 | 0.00000 |
| 802 | 82 | ILE | CB | -12.60010 | -11.87598 | 93.53959 | A1 | 82 | 0.00000 |
| 803 | 82 | ILE | CG2 | -12.41140 | -13.13773 | 94.38674 | A1 | 82 | 0.00000 |
| 804 | 82 | ILE | CG1 | -11.31152 | -11.05228 | 93.44331 | A1 | 82 | 0.00000 |
| 805 | 82 | ILE | CD | -10.76554 | -10.62709 | 94.80896 | A1 | 82 | 0.00000 |
| 806 | 82 | ILE | C | -12.35649 | -13.19907 | 91.37376 | A1 | 82 | 0.00000 |
| 807 | 82 | ILE | OCT1 | -11.36717 | -12.81747 | 90.75062 | A1 | 82 | 0.00000 |
| 808 | 82 | ILE | OCT2 | -12.72556 | -14.37446 | 91.38671 | A1 | 82 | 0.00000 |
| 809 | 83 | GLY | N | -17.53322 | -0.31236 | 94.99084 | B1 | 1 | 0.00000 |
| 810 | 83 | GLY | HT1 | -17.21994 | 0.44323 | 94.35235 | B1 | 1 | 0.00000 |
| 811 | 83 | GLY | HT2 | -16.86357 | -1.12219 | 94.96444 | B1 | 1 | 0.00000 |
| 812 | 83 | GLY | HT3 | -17.61098 | 0.01920 | 95.97150 | B1 | 1 | 0.00000 |
| 813 | 83 | GLY | CA | -18.79853 | -0.91116 | 94.55151 | B1 | 1 | 0.00000 |
| 814 | 83 | GLY | C | -18.62573 | -2.38203 | 94.66351 | B1 | 1 | 0.00000 |
| 815 | 83 | GLY | O | -17.35786 | -2.70920 | 94.84086 | B1 | 1 | 0.00000 |
| 816 | 84 | ASP | N | -19.57260 | -3.20239 | 94.59303 | B1 | 2 | 0.00000 |
| 817 | 84 | ASP | H | -20.49658 | -2.89510 | 94.35600 | B1 | 2 | 0.00000 |
| 818 | 84 | ASP | CA | -19.43900 | -4.63200 | 94.86181 | B1 | 2 | 0.00000 |
| 819 | 84 | ASP | CB | -19.44643 | -4.83356 | 96.38475 | B1 | 2 | 0.00000 |
| 820 | 84 | ASP | CG | -18.89301 | -6.19619 | 96.73815 | B1 | 2 | 0.00000 |
| 821 | 84 | ASP | OD1 | -17.69451 | -6.29764 | 96.98109 | B1 | 2 | 0.00000 |
| 822 | 84 | ASP | OD2 | -19.66566 | -7.14958 | 96.75715 | B1 | 2 | 0.00000 |
| 823 | 84 | ASP | C | -20.62786 | -5.31072 | 94.19848 | B1 | 2 | 0.00000 |
| 824 | 84 | ASP | O | -21.46903 | -4.61697 | 93.63479 | B1 | 2 | 0.00000 |
| 825 | 85 | THR | N | -20.67796 | -6.64606 | 94.24891 | B1 | 3 | 0.00000 |
| 826 | 85 | THR | H | -20.04362 | -7.15926 | 94.84032 | B1 | 3 | 0.00000 |
| 827 | 85 | THR | CA | -21.75257 | -7.39367 | 93.59154 | B1 | 3 | 0.00000 |
| 828 | 85 | THR | CB | -21.58903 | -7.31950 | 92.05122 | B1 | 3 | 0.00000 |

FIG. 14

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 829 | 85 | THR | OG1 | 22.76265 | -7.82480 | 91.39964 | B1 | 3 | 0.00000 |
| 830 | 85 | THR | HG1 | -22.73431 | -7.60152 | 90.46343 | B1 | 3 | 0.00000 |
| 831 | 85 | THR | CG2 | -20.32966 | -8.02078 | 91.53071 | B1 | 3 | 0.00000 |
| 832 | 85 | THR | C | -21.74290 | -8.83241 | 94.09035 | B1 | 3 | 0.00000 |
| 833 | 85 | THR | O | -20.76454 | -9.30377 | 94.65381 | B1 | 3 | 0.00000 |
| 834 | 86 | ARG | N | -22.86491 | -9.52779 | 93.88799 | B1 | 4 | 0.00000 |
| 835 | 86 | ARG | H | -23.62404 | -9.13760 | 93.36423 | B1 | 4 | 0.00000 |
| 836 | 86 | ARG | CA | -22.93360 | -10.87552 | 94.44830 | B1 | 4 | 0.00000 |
| 837 | 86 | ARG | CB | -23.51668 | -10.79083 | 95.86916 | B1 | 4 | 0.00000 |
| 838 | 86 | ARG | CG | -22.74323 | -11.65365 | 96.87092 | B1 | 4 | 0.00000 |
| 839 | 86 | ARG | CD | -23.23116 | -13.10294 | 97.02541 | B1 | 4 | 0.00000 |
| 840 | 86 | ARG | NE | -22.12580 | -14.03911 | 97.27083 | B1 | 4 | 0.00000 |
| 841 | 86 | ARG | HE | -21.93083 | -14.68836 | 96.53494 | B1 | 4 | 0.00000 |
| 842 | 86 | ARG | CZ | -21.37502 | -14.05016 | 98.38612 | B1 | 4 | 0.00000 |
| 843 | 86 | ARG | NH1 | -20.31371 | -14.85617 | 98.44757 | B1 | 4 | 0.00000 |
| 844 | 86 | ARG | HH11 | -19.73815 | -14.87872 | 99.26299 | B1 | 4 | 0.00000 |
| 845 | 86 | ARG | HH12 | -20.05194 | -15.47498 | 97.69021 | B1 | 4 | 0.00000 |
| 846 | 86 | ARG | NH2 | -21.67517 | -13.26636 | 99.42563 | B1 | 4 | 0.00000 |
| 847 | 86 | ARG | HH21 | -21.13780 | -13.26659 | 100.26897 | B1 | 4 | 0.00000 |
| 848 | 86 | ARG | HH22 | -22.46145 | -12.65025 | 99.36831 | B1 | 4 | 0.00000 |
| 849 | 86 | ARG | C | -23.73522 | -11.82065 | 93.57905 | B1 | 4 | 0.00000 |
| 850 | 86 | ARG | O | -24.85200 | -11.52803 | 93.17882 | B1 | 4 | 0.00000 |
| 851 | 87 | PRO | N | -23.12190 | -12.98532 | 93.27325 | B1 | 5 | 0.00000 |
| 852 | 87 | PRO | CD | -21.73269 | -13.34562 | 93.54376 | B1 | 5 | 0.00000 |
| 853 | 87 | PRO | CA | -23.84439 | -14.02757 | 92.53087 | B1 | 5 | 0.00000 |
| 854 | 87 | PRO | CB | -22.78528 | -15.13066 | 92.39999 | B1 | 5 | 0.00000 |
| 855 | 87 | PRO | CG | -21.43460 | -14.43376 | 92.52460 | B1 | 5 | 0.00000 |
| 856 | 87 | PRO | C | -25.10390 | -14.54496 | 93.21975 | B1 | 5 | 0.00000 |
| 857 | 87 | PRO | O | -25.32441 | -14.39544 | 94.41838 | B1 | 5 | 0.00000 |
| 858 | 88 | ARG | N | -25.94344 | -15.17061 | 92.39123 | B1 | 6 | 0.00000 |
| 859 | 88 | ARG | H | -25.68611 | -15.35588 | 91.44433 | B1 | 6 | 0.00000 |
| 860 | 88 | ARG | CA | -27.23219 | -15.62675 | 92.90235 | B1 | 6 | 0.00000 |
| 861 | 88 | ARG | CB | -28.29078 | -15.39805 | 91.81653 | B1 | 6 | 0.00000 |
| 862 | 88 | ARG | CG | -29.70863 | -15.55859 | 92.35844 | B1 | 6 | 0.00000 |
| 863 | 88 | ARG | CD | -30.79150 | -14.91787 | 91.49236 | B1 | 6 | 0.00000 |
| 864 | 88 | ARG | NE | -31.92741 | -14.57277 | 92.34607 | B1 | 6 | 0.00000 |
| 865 | 88 | ARG | HE | -31.76512 | -14.64038 | 93.33788 | B1 | 6 | 0.00000 |
| 866 | 88 | ARG | CZ | -33.08881 | -14.12165 | 91.86193 | B1 | 6 | 0.00000 |
| 867 | 88 | ARG | NH1 | -34.06565 | -13.81756 | 92.71322 | B1 | 6 | 0.00000 |
| 868 | 88 | ARG | HH11 | -34.95441 | -13.48197 | 92.40144 | B1 | 6 | 0.00000 |
| 869 | 88 | ARG | HH12 | -33.91853 | -13.92533 | 93.69838 | B1 | 6 | 0.00000 |
| 870 | 88 | ARG | NH2 | -33.26623 | -13.97383 | 90.54974 | B1 | 6 | 0.00000 |
| 871 | 88 | ARG | HH21 | -34.12737 | -13.64013 | 90.16725 | B1 | 6 | 0.00000 |
| 872 | 88 | ARG | HH22 | -32.52080 | -14.19859 | 89.92214 | B1 | 6 | 0.00000 |
| 873 | 88 | ARG | C | -27.23157 | -17.07404 | 93.36366 | B1 | 6 | 0.00000 |
| 874 | 88 | ARG | O | -26.89591 | -18.00090 | 92.63574 | B1 | 6 | 0.00000 |
| 875 | 89 | PHE | N | -27.62757 | -17.24057 | 94.62546 | B1 | 7 | 0.00000 |
| 876 | 89 | PHE | H | -27.92346 | -16.46797 | 95.18173 | B1 | 7 | 0.00000 |
| 877 | 89 | PHE | CA | -27.64368 | -18.59443 | 95.17433 | B1 | 7 | 0.00000 |
| 878 | 89 | PHE | CB | -26.56379 | -18.74887 | 96.25427 | B1 | 7 | 0.00000 |
| 879 | 89 | PHE | CG | -25.20774 | -18.55805 | 95.61829 | B1 | 7 | 0.00000 |
| 880 | 89 | PHE | CD1 | -24.74915 | -19.48139 | 94.64858 | B1 | 7 | 0.00000 |
| 881 | 89 | PHE | CD2 | -24.42840 | -17.43023 | 95.96102 | B1 | 7 | 0.00000 |
| 882 | 89 | PHE | CE1 | -23.51045 | -19.27079 | 94.00961 | B1 | 7 | 0.00000 |
| 883 | 89 | PHE | CE2 | -23.18767 | -17.21976 | 95.32384 | B1 | 7 | 0.00000 |
| 884 | 89 | PHE | CZ | -22.73800 | -18.13927 | 94.34976 | B1 | 7 | 0.00000 |
| 885 | 89 | PHE | C | -28.99632 | -18.97147 | 95.72084 | B1 | 7 | 0.00000 |
| 886 | 89 | PHE | O | -29.85551 | -18.12429 | 95.94786 | B1 | 7 | 0.00000 |
| 887 | 90 | LEU | N | -29.15750 | -20.28822 | 95.87791 | B1 | 8 | 0.00000 |
| 888 | 90 | LEU | H | -28.38720 | -20.92114 | 95.76376 | B1 | 8 | 0.00000 |
| 889 | 90 | LEU | CA | -30.48975 | -20.82226 | 96.14113 | B1 | 8 | 0.00000 |
| 890 | 90 | LEU | CB | -31.01266 | -21.46546 | 94.84981 | B1 | 8 | 0.00000 |
| 891 | 90 | LEU | CG | -32.46079 | -21.16892 | 94.43614 | B1 | 8 | 0.00000 |
| 892 | 90 | LEU | CD1 | -32.81137 | -21.98230 | 93.19113 | B1 | 8 | 0.00000 |

FIG. 15

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 15

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 893 | 90 | LEU | CD2 | 3.47498 | -21.40699 | 95.55222 | B1 | 8 | 0.00000 |
| 894 | 90 | LEU | C | -30.45467 | -21.90281 | 97.20252 | B1 | 8 | 0.00000 |
| 895 | 90 | LEU | O | -29.74216 | -22.89200 | 97.07224 | B1 | 8 | 0.00000 |
| 896 | 91 | TRP | N | -31.28133 | -21.71086 | 98.22982 | B1 | 9 | 0.00000 |
| 897 | 91 | TRP | H | -31.78897 | -20.85226 | 98.31900 | B1 | 9 | 0.00000 |
| 898 | 91 | TRP | CA | -31.61477 | -22.86043 | 99.06700 | B1 | 9 | 0.00000 |
| 899 | 91 | TRP | CB | -31.76159 | -22.50789 | 100.54418 | B1 | 9 | 0.00000 |
| 900 | 91 | TRP | CG | -30.46050 | -22.11490 | 101.18157 | B1 | 9 | 0.00000 |
| 901 | 91 | TRP | CD2 | -29.22893 | -22.79283 | 101.16170 | B1 | 9 | 0.00000 |
| 902 | 91 | TRP | CE2 | -28.30074 | -21.96546 | 101.98847 | B1 | 9 | 0.00000 |
| 903 | 91 | TRP | CE3 | -28.77368 | -24.00327 | 100.60389 | B1 | 9 | 0.00000 |
| 904 | 91 | TRP | CD1 | -30.26500 | -20.96427 | 101.96112 | B1 | 9 | 0.00000 |
| 905 | 91 | TRP | NE1 | -28.99810 | -20.87047 | 102.44030 | B1 | 9 | 0.00000 |
| 906 | 91 | TRP | HE1 | -28.68566 | -20.15616 | 103.04137 | B1 | 9 | 0.00000 |
| 907 | 91 | TRP | CZ2 | -26.97767 | -22.40520 | 102.16578 | B1 | 9 | 0.00000 |
| 908 | 91 | TRP | CZ3 | -27.44054 | -24.40402 | 100.81577 | B1 | 9 | 0.00000 |
| 909 | 91 | TRP | CH2 | -26.56124 | -23.61859 | 101.58828 | B1 | 9 | 0.00000 |
| 910 | 91 | TRP | C | -32.96765 | -23.39534 | 98.70806 | B1 | 9 | 0.00000 |
| 911 | 91 | TRP | O | -33.92486 | -22.66026 | 98.49798 | B1 | 9 | 0.00000 |
| 912 | 92 | GLN | N | -33.02847 | -24.71550 | 98.69197 | B1 | 10 | 0.00000 |
| 913 | 92 | GLN | H | -32.20362 | -25.28365 | 98.76579 | B1 | 10 | 0.00000 |
| 914 | 92 | GLN | CA | -34.33516 | -25.34751 | 98.65309 | B1 | 10 | 0.00000 |
| 915 | 92 | GLN | CB | -34.50105 | -26.04119 | 97.30049 | B1 | 10 | 0.00000 |
| 916 | 92 | GLN | CG | -34.43287 | -25.05724 | 96.13126 | B1 | 10 | 0.00000 |
| 917 | 92 | GLN | CD | -34.12668 | -25.79390 | 94.84833 | B1 | 10 | 0.00000 |
| 918 | 92 | GLN | OE1 | -32.99424 | -25.88838 | 94.39010 | B1 | 10 | 0.00000 |
| 919 | 92 | GLN | NE2 | -35.19268 | -26.32196 | 94.25873 | B1 | 10 | 0.00000 |
| 920 | 92 | GLN | HE21 | -36.10617 | -26.21874 | 94.65013 | B1 | 10 | 0.00000 |
| 921 | 92 | GLN | HE22 | -35.08609 | -26.83019 | 93.40658 | B1 | 10 | 0.00000 |
| 922 | 92 | GLN | C | -34.37000 | -26.35610 | 99.77327 | B1 | 10 | 0.00000 |
| 923 | 92 | GLN | O | -33.40619 | -27.07419 | 100.00960 | B1 | 10 | 0.00000 |
| 924 | 93 | LEU | N | -35.49484 | -26.39205 | 100.47380 | B1 | 11 | 0.00000 |
| 925 | 93 | LEU | H | -36.24432 | -25.74963 | 100.29272 | B1 | 11 | 0.00000 |
| 926 | 93 | LEU | CA | -35.59559 | -27.43909 | 101.48633 | B1 | 11 | 0.00000 |
| 927 | 93 | LEU | CB | -35.41178 | -26.81504 | 102.88181 | B1 | 11 | 0.00000 |
| 928 | 93 | LEU | CG | -34.83577 | -27.70766 | 103.99848 | B1 | 11 | 0.00000 |
| 929 | 93 | LEU | CD1 | -34.33031 | -26.83824 | 105.14843 | B1 | 11 | 0.00000 |
| 930 | 93 | LEU | CD2 | -35.82812 | -28.74167 | 104.52805 | B1 | 11 | 0.00000 |
| 931 | 93 | LEU | C | -36.93596 | -28.11112 | 101.32695 | B1 | 11 | 0.00000 |
| 932 | 93 | LEU | O | -37.91692 | -27.47571 | 100.96621 | B1 | 11 | 0.00000 |
| 933 | 94 | LYS | N | -36.95045 | -29.41719 | 101.56549 | B1 | 12 | 0.00000 |
| 934 | 94 | LYS | H | -36.10205 | -29.89066 | 101.79736 | B1 | 12 | 0.00000 |
| 935 | 94 | LYS | CA | -38.21063 | -30.14121 | 101.49214 | B1 | 12 | 0.00000 |
| 936 | 94 | LYS | CB | -38.26049 | -30.88530 | 100.13839 | B1 | 12 | 0.00000 |
| 937 | 94 | LYS | CG | -39.43761 | -31.85442 | 100.07544 | B1 | 12 | 0.00000 |
| 938 | 94 | LYS | CD | -39.91969 | -32.44832 | 98.75113 | B1 | 12 | 0.00000 |
| 939 | 94 | LYS | CE | -41.00198 | -33.40442 | 99.23924 | B1 | 12 | 0.00000 |
| 940 | 94 | LYS | NZ | -41.98389 | -33.90963 | 98.26846 | B1 | 12 | 0.00000 |
| 941 | 94 | LYS | HZ1 | -42.69798 | -34.41995 | 98.86351 | B1 | 12 | 0.00000 |
| 942 | 94 | LYS | HZ2 | -42.49249 | -33.14263 | 97.78947 | B1 | 12 | 0.00000 |
| 943 | 94 | LYS | HZ3 | -41.57162 | -34.57937 | 97.59540 | B1 | 12 | 0.00000 |
| 944 | 94 | LYS | C | -38.34910 | -31.08699 | 102.67642 | B1 | 12 | 0.00000 |
| 945 | 94 | LYS | O | -37.54720 | -31.99770 | 102.85849 | B1 | 12 | 0.00000 |
| 946 | 95 | PHE | N | -39.40676 | -30.85929 | 103.46609 | B1 | 13 | 0.00000 |
| 947 | 95 | PHE | H | -39.99321 | -30.05201 | 103.34519 | B1 | 13 | 0.00000 |
| 948 | 95 | PHE | CA | -39.73794 | -31.84982 | 104.49053 | B1 | 13 | 0.00000 |
| 949 | 95 | PHE | CB | -39.13251 | -31.49228 | 105.86481 | B1 | 13 | 0.00000 |
| 950 | 95 | PHE | CG | -39.62104 | -30.20819 | 106.49960 | B1 | 13 | 0.00000 |
| 951 | 95 | PHE | CD1 | -39.04917 | -28.96886 | 106.12996 | B1 | 13 | 0.00000 |
| 952 | 95 | PHE | CD2 | -40.60668 | -30.26479 | 107.51173 | B1 | 13 | 0.00000 |
| 953 | 95 | PHE | CE1 | -39.45587 | -27.78326 | 106.77985 | B1 | 13 | 0.00000 |
| 954 | 95 | PHE | CE2 | -41.01477 | -29.08019 | 108.16313 | B1 | 13 | 0.00000 |
| 955 | 95 | PHE | CZ | -40.43557 | -27.84435 | 107.79605 | B1 | 13 | 0.00000 |
| 956 | 95 | PHE | C | -41.22005 | -32.16799 | 104.57423 | B1 | 13 | 0.00000 |

FIG. 16

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 957 | 95 | PHE | O | - .08591 | -31.31332 | 104.41691 | B1 | 13 | -0.00000 |
| 958 | 96 | GLU | N | -..47812 | -33.46734 | 104.75822 | B1 | 14 | 0.00000 |
| 959 | 96 | GLU | H | -40.74093 | -34.09071 | 105.01948 | B1 | 14 | 0.00000 |
| 960 | 96 | GLU | CA | -42.80002 | -33.99059 | 104.40078 | B1 | 14 | 0.00000 |
| 961 | 96 | GLU | CB | -42.75085 | -34.25375 | 102.88321 | B1 | 14 | 0.00000 |
| 962 | 96 | GLU | CG | -43.92070 | -34.87965 | 102.11791 | B1 | 14 | 0.00000 |
| 963 | 96 | GLU | CD | -43.55505 | -34.92496 | 100.64018 | B1 | 14 | 0.00000 |
| 964 | 96 | GLU | OE1 | -44.08205 | -34.15253 | 99.84297 | B1 | 14 | 0.00000 |
| 965 | 96 | GLU | OE2 | -42.67962 | -35.68559 | 100.23154 | B1 | 14 | 0.00000 |
| 966 | 96 | GLU | C | -43.13129 | -35.25393 | 105.17925 | B1 | 14 | 0.00000 |
| 967 | 96 | GLU | O | -42.27510 | -36.11395 | 105.37879 | B1 | 14 | 0.00000 |
| 968 | 97 | CYS | N | -44.39621 | -35.34431 | 105.62501 | B1 | 15 | 0.00000 |
| 969 | 97 | CYS | H | -45.05281 | -34.60566 | 105.44206 | B1 | 15 | 0.00000 |
| 970 | 97 | CYS | CA | -44.78990 | -36.60747 | 106.25700 | B1 | 15 | 0.00000 |
| 971 | 97 | CYS | CB | -45.09404 | -36.46870 | 107.76554 | B1 | 15 | 0.00000 |
| 972 | 97 | CYS | SG | -46.49873 | -35.54248 | 108.42288 | B1 | 15 | 0.00000 |
| 973 | 97 | CYS | C | -45.89248 | -37.36966 | 105.55706 | B1 | 15 | 0.00000 |
| 974 | 97 | CYS | O | -46.75253 | -36.80546 | 104.88787 | B1 | 15 | 0.00000 |
| 975 | 98 | HIS | N | -45.80356 | -38.69951 | 105.71784 | B1 | 16 | 0.00000 |
| 976 | 98 | HIS | H | -45.06854 | -39.11332 | 106.26371 | B1 | 16 | 0.00000 |
| 977 | 98 | HIS | CA | -46.75592 | -39.59530 | 105.05785 | B1 | 16 | 0.00000 |
| 978 | 98 | HIS | CB | -46.00867 | -40.61029 | 104.19437 | B1 | 16 | 0.00000 |
| 979 | 98 | HIS | CG | -45.38253 | -39.98357 | 102.97364 | B1 | 16 | 0.00000 |
| 980 | 98 | HIS | ND1 | -45.88967 | -40.13539 | 101.74183 | B1 | 16 | 0.00000 |
| 981 | 98 | HIS | HD1 | -46.72307 | -40.60043 | 101.51181 | B1 | 16 | 0.00000 |
| 982 | 98 | HIS | CD2 | -44.21286 | -39.22166 | 102.89430 | B1 | 16 | 0.00000 |
| 983 | 98 | HIS | NE2 | -44.02278 | -38.92334 | 101.58753 | B1 | 16 | 0.00000 |
| 984 | 98 | HIS | CE1 | -45.05268 | -39.48082 | 100.87633 | B1 | 16 | 0.00000 |
| 985 | 98 | HIS | C | -47.56750 | -40.40062 | 106.05217 | B1 | 16 | 0.00000 |
| 986 | 98 | HIS | O | -47.04279 | -40.99638 | 106.99225 | B1 | 16 | 0.00000 |
| 987 | 99 | PHE | N | -48.87987 | -40.39547 | 105.81218 | B1 | 17 | 0.00000 |
| 988 | 99 | PHE | H | -49.25243 | -39.92869 | 105.00666 | B1 | 17 | 0.00000 |
| 989 | 99 | PHE | CA | -49.78029 | -41.01889 | 106.77662 | B1 | 17 | 0.00000 |
| 990 | 99 | PHE | CB | -50.48946 | -39.93190 | 107.59234 | B1 | 17 | 0.00000 |
| 991 | 99 | PHE | CG | -49.63868 | -39.72312 | 108.81497 | B1 | 17 | 0.00000 |
| 992 | 99 | PHE | CD1 | -48.50685 | -38.87580 | 108.76543 | B1 | 17 | 0.00000 |
| 993 | 99 | PHE | CD2 | -49.92563 | -40.47457 | 109.97439 | B1 | 17 | 0.00000 |
| 994 | 99 | PHE | CE1 | -47.64103 | -38.80002 | 109.87537 | B1 | 17 | 0.00000 |
| 995 | 99 | PHE | CE2 | -49.06252 | -40.39779 | 111.08354 | B1 | 17 | 0.00000 |
| 996 | 99 | PHE | CZ | -47.92137 | -39.56658 | 111.02626 | B1 | 17 | 0.00000 |
| 997 | 99 | PHE | C | -50.79242 | -41.97404 | 106.19800 | B1 | 17 | 0.00000 |
| 998 | 99 | PHE | O | -51.48007 | -41.71068 | 105.22101 | B1 | 17 | 0.00000 |
| 999 | 100 | PHE | N | -50.86837 | -43.12653 | 106.85844 | B1 | 18 | 0.00000 |
| 1000 | 100 | PHE | H | -50.32768 | -43.27017 | 107.68944 | B1 | 18 | 0.00000 |
| 1001 | 100 | PHE | CA | -51.84718 | -44.10783 | 106.41132 | B1 | 18 | 0.00000 |
| 1002 | 100 | PHE | CB | -51.44468 | -45.52210 | 106.84262 | B1 | 18 | 0.00000 |
| 1003 | 100 | PHE | CG | -51.08740 | -46.34931 | 105.63001 | B1 | 18 | 0.00000 |
| 1004 | 100 | PHE | CD1 | -49.81159 | -46.95065 | 105.55366 | B1 | 18 | 0.00000 |
| 1005 | 100 | PHE | CD2 | -52.01269 | -46.50158 | 104.56911 | B1 | 18 | 0.00000 |
| 1006 | 100 | PHE | CE1 | -49.45012 | -47.69723 | 104.41336 | B1 | 18 | 0.00000 |
| 1007 | 100 | PHE | CE2 | -51.65494 | -47.24829 | 103.42719 | B1 | 18 | 0.00000 |
| 1008 | 100 | PHE | CZ | -50.37408 | -47.83859 | 103.35608 | B1 | 18 | 0.00000 |
| 1009 | 100 | PHE | C | -53.21727 | -43.84401 | 106.96975 | B1 | 18 | 0.00000 |
| 1010 | 100 | PHE | O | -53.38235 | -43.49692 | 108.13319 | B1 | 18 | 0.00000 |
| 1011 | 101 | ASN | N | -54.19611 | -44.08275 | 106.08672 | B1 | 19 | 0.00000 |
| 1012 | 101 | ASN | H | -53.92777 | -44.28429 | 105.14366 | B1 | 19 | 0.00000 |
| 1013 | 101 | ASN | CA | -55.63451 | -43.97453 | 106.37273 | B1 | 19 | 0.00000 |
| 1014 | 101 | ASN | CB | -56.35400 | -45.03359 | 105.52094 | B1 | 19 | 0.00000 |
| 1015 | 101 | ASN | CG | -57.86040 | -44.83624 | 105.52911 | B1 | 19 | 0.00000 |
| 1016 | 101 | ASN | OD1 | -58.43246 | -44.06601 | 104.77523 | B1 | 19 | 0.00000 |
| 1017 | 101 | ASN | ND2 | -58.51327 | -45.58184 | 106.41359 | B1 | 19 | 0.00000 |
| 1018 | 101 | ASN | HD21 | -58.04843 | -46.21753 | 107.02623 | B1 | 19 | 0.00000 |
| 1019 | 101 | ASN | HD22 | -59.50666 | -45.49785 | 106.46882 | B1 | 19 | 0.00000 |
| 1020 | 101 | ASN | C | -56.06277 | -44.09262 | 107.83398 | B1 | 19 | 0.00000 |

FIG. 17

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1021 | 101 | ASN | O | -56.73737 | -43.23997 | 108.39463 | B1 | 19 | 0.00000 |
| 1022 | 102 | GLY | N | -55.63460 | -45.10941 | 108.46454 | B1 | 20 | 0.00000 |
| 1023 | 102 | GLY | H | -55.00370 | -45.02188 | 108.01935 | B1 | 20 | 0.00000 |
| 1024 | 102 | GLY | CA | -55.97438 | -45.32353 | 109.88157 | B1 | 20 | 0.00000 |
| 1025 | 102 | GLY | C | -55.02088 | -44.59872 | 110.81953 | B1 | 20 | 0.00000 |
| 1026 | 102 | GLY | O | -54.46008 | -45.17864 | 111.73800 | B1 | 20 | 0.00000 |
| 1027 | 103 | THR | N | -54.84744 | -43.29716 | 110.54648 | B1 | 21 | 0.00000 |
| 1028 | 103 | THR | H | -55.35512 | -42.90731 | 109.77435 | B1 | 21 | 0.00000 |
| 1029 | 103 | THR | CA | -53.96549 | -42.39542 | 111.30363 | B1 | 21 | 0.00000 |
| 1030 | 103 | THR | CB | -54.75487 | -41.81263 | 112.51011 | B1 | 21 | 0.00000 |
| 1031 | 103 | THR | OG1 | -54.22405 | -40.53356 | 112.87483 | B1 | 21 | 0.00000 |
| 1032 | 103 | THR | HG1 | -54.81974 | -40.09919 | 113.49221 | B1 | 21 | 0.00000 |
| 1033 | 103 | THR | CG2 | -54.86925 | -42.72433 | 113.73959 | B1 | 21 | 0.00000 |
| 1034 | 103 | THR | C | -52.56983 | -42.92386 | 111.66956 | B1 | 21 | 0.00000 |
| 1035 | 103 | THR | O | -51.96086 | -42.59288 | 112.68707 | B1 | 21 | 0.00000 |
| 1036 | 104 | GLU | N | -52.05837 | -43.78433 | 110.78327 | B1 | 22 | 0.00000 |
| 1037 | 104 | GLU | H | -52.50836 | -43.94021 | 109.90068 | B1 | 22 | 0.00000 |
| 1038 | 104 | GLU | CA | -50.80234 | -44.42458 | 111.16198 | B1 | 22 | 0.00000 |
| 1039 | 104 | GLU | CB | -50.88647 | -45.95191 | 111.05395 | B1 | 22 | 0.00000 |
| 1040 | 104 | GLU | CG | -51.13368 | -46.62525 | 112.41591 | B1 | 22 | 0.00000 |
| 1041 | 104 | GLU | CD | -50.07267 | -46.21410 | 113.43075 | B1 | 22 | 0.00000 |
| 1042 | 104 | GLU | OE1 | -50.42273 | -45.91599 | 114.57130 | B1 | 22 | 0.00000 |
| 1043 | 104 | GLU | OE2 | -48.89658 | -46.13148 | 113.08359 | B1 | 22 | 0.00000 |
| 1044 | 104 | GLU | C | -49.56607 | -43.91901 | 110.45954 | B1 | 22 | 0.00000 |
| 1045 | 104 | GLU | O | -49.58628 | -43.40196 | 109.34894 | B1 | 22 | 0.00000 |
| 1046 | 105 | ARG | N | -48.46470 | -44.04978 | 111.19345 | B1 | 23 | 0.00000 |
| 1047 | 105 | ARG | H | -48.46820 | -44.67995 | 111.97754 | B1 | 23 | 0.00000 |
| 1048 | 105 | ARG | CA | -47.23862 | -43.36578 | 110.79677 | B1 | 23 | 0.00000 |
| 1049 | 105 | ARG | CB | -46.43619 | -43.14957 | 112.09184 | B1 | 23 | 0.00000 |
| 1050 | 105 | ARG | CG | -45.11167 | -42.37595 | 112.05228 | B1 | 23 | 0.00000 |
| 1051 | 105 | ARG | CD | -43.89570 | -43.22016 | 111.65081 | B1 | 23 | 0.00000 |
| 1052 | 105 | ARG | NE | -42.65640 | -42.48704 | 111.89499 | B1 | 23 | 0.00000 |
| 1053 | 105 | ARG | HE | -42.30777 | -42.45915 | 112.83941 | B1 | 23 | 0.00000 |
| 1054 | 105 | ARG | CZ | -42.05554 | -41.77685 | 110.93892 | B1 | 23 | 0.00000 |
| 1055 | 105 | ARG | NH1 | -41.02352 | -41.00938 | 111.25165 | B1 | 23 | 0.00000 |
| 1056 | 105 | ARG | HH11 | -40.51476 | -40.49136 | 110.56874 | B1 | 23 | 0.00000 |
| 1057 | 105 | ARG | HH12 | -40.73208 | -40.92747 | 112.21979 | B1 | 23 | 0.00000 |
| 1058 | 105 | ARG | NH2 | -42.47661 | -41.82718 | 109.68286 | B1 | 23 | 0.00000 |
| 1059 | 105 | ARG | HH21 | -42.19810 | -41.15340 | 109.00310 | B1 | 23 | 0.00000 |
| 1060 | 105 | ARG | HH22 | -43.08503 | -42.57763 | 109.38941 | B1 | 23 | 0.00000 |
| 1061 | 105 | ARG | C | -46.47373 | -44.13883 | 109.74376 | B1 | 23 | 0.00000 |
| 1062 | 105 | ARG | O | -46.02105 | -45.25363 | 109.97034 | B1 | 23 | 0.00000 |
| 1063 | 106 | VAL | N | -46.32883 | -43.51517 | 108.56827 | B1 | 24 | 0.00000 |
| 1064 | 106 | VAL | H | -46.72693 | -42.61352 | 108.37187 | B1 | 24 | 0.00000 |
| 1065 | 106 | VAL | CA | -45.53349 | -44.24499 | 107.58352 | B1 | 24 | 0.00000 |
| 1066 | 106 | VAL | CB | -46.27081 | -44.39073 | 106.24298 | B1 | 24 | 0.00000 |
| 1067 | 106 | VAL | CG1 | -45.79579 | -45.65575 | 105.52366 | B1 | 24 | 0.00000 |
| 1068 | 106 | VAL | CG2 | -47.77990 | -44.41166 | 106.42922 | B1 | 24 | 0.00000 |
| 1069 | 106 | VAL | C | -44.14065 | -43.66075 | 107.41554 | B1 | 24 | 0.00000 |
| 1070 | 106 | VAL | O | -43.30354 | -43.80891 | 108.29696 | B1 | 24 | 0.00000 |
| 1071 | 107 | ARG | N | -43.87314 | -42.98069 | 106.29416 | B1 | 25 | 0.00000 |
| 1072 | 107 | ARG | H | -44.58452 | -42.69040 | 105.65671 | B1 | 25 | 0.00000 |
| 1073 | 107 | ARG | CA | -42.49561 | -42.53115 | 106.12329 | B1 | 25 | 0.00000 |
| 1074 | 107 | ARG | CB | -41.95685 | -43.01317 | 104.76032 | B1 | 25 | 0.00000 |
| 1075 | 107 | ARG | CG | -41.96328 | -42.02619 | 103.58362 | B1 | 25 | 0.00000 |
| 1076 | 107 | ARG | CD | -42.33357 | -42.66829 | 102.24883 | B1 | 25 | 0.00000 |
| 1077 | 107 | ARG | NE | -43.76838 | -42.93515 | 102.23147 | B1 | 25 | 0.00000 |
| 1078 | 107 | ARG | HE | -44.37946 | -42.14312 | 102.28284 | B1 | 25 | 0.00000 |
| 1079 | 107 | ARG | CZ | -44.26510 | -44.17490 | 102.20945 | B1 | 25 | 0.00000 |
| 1080 | 107 | ARG | NH1 | -45.56598 | -44.32747 | 102.35905 | B1 | 25 | 0.00000 |
| 1081 | 107 | ARG | HH11 | -46.08629 | -45.19207 | 102.34562 | B1 | 25 | 0.00000 |
| 1082 | 107 | ARG | HH12 | -46.19539 | -43.55730 | 102.54612 | B1 | 25 | 0.00000 |
| 1083 | 107 | ARG | NH2 | -43.47983 | -45.23695 | 102.05798 | B1 | 25 | 0.00000 |
| 1084 | 107 | ARG | HH21 | -43.86541 | -46.15896 | 102.05452 | B1 | 25 | 0.00000 |

FIG. 18

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1085 | 107 | ARG | HH22 | 2.49404 | -45.11997 | 101.94496 | B1 | 25 | 0.00000 |
| 1086 | 107 | ARG | C | -42.37787 | -41.03546 | 106.32504 | B1 | 25 | 0.00000 |
| 1087 | 107 | ARG | O | -43.36896 | -40.31981 | 106.43645 | B1 | 25 | 0.00000 |
| 1088 | 108 | LEU | N | -41.12633 | -40.58602 | 106.39627 | B1 | 26 | 0.00000 |
| 1089 | 108 | LEU | H | -40.32617 | -41.17985 | 106.29320 | B1 | 26 | 0.00000 |
| 1090 | 108 | LEU | CA | -40.89942 | -39.15744 | 106.53751 | B1 | 26 | 0.00000 |
| 1091 | 108 | LEU | CB | -40.80087 | -38.80954 | 108.01248 | B1 | 26 | 0.00000 |
| 1092 | 108 | LEU | CG | -41.96347 | -37.89689 | 108.35874 | B1 | 26 | 0.00000 |
| 1093 | 108 | LEU | CD1 | -42.75820 | -38.44729 | 109.53808 | B1 | 26 | 0.00000 |
| 1094 | 108 | LEU | CD2 | -41.50070 | -36.44650 | 108.50151 | B1 | 26 | 0.00000 |
| 1095 | 108 | LEU | C | -39.62061 | -38.77273 | 105.85764 | B1 | 26 | 0.00000 |
| 1096 | 108 | LEU | O | -38.76368 | -39.61093 | 105.60154 | B1 | 26 | 0.00000 |
| 1097 | 109 | LEU | N | -39.52150 | -37.47828 | 105.56773 | B1 | 27 | 0.00000 |
| 1098 | 109 | LEU | H | -40.28459 | -36.84167 | 105.72467 | B1 | 27 | 0.00000 |
| 1099 | 109 | LEU | CA | -38.30683 | -37.02679 | 104.90334 | B1 | 27 | 0.00000 |
| 1100 | 109 | LEU | CB | -38.47418 | -37.24039 | 103.39009 | B1 | 27 | 0.00000 |
| 1101 | 109 | LEU | CG | -39.74490 | -36.59695 | 102.82634 | B1 | 27 | 0.00000 |
| 1102 | 109 | LEU | CD1 | -39.42210 | -35.25631 | 102.17066 | B1 | 27 | 0.00000 |
| 1103 | 109 | LEU | CD2 | -40.49190 | -37.56523 | 101.91138 | B1 | 27 | 0.00000 |
| 1104 | 109 | LEU | C | -37.99969 | -35.58061 | 105.21268 | B1 | 27 | 0.00000 |
| 1105 | 109 | LEU | O | -38.88411 | -34.77322 | 105.47943 | B1 | 27 | 0.00000 |
| 1106 | 110 | GLU | N | -36.70092 | -35.29768 | 105.12126 | B1 | 28 | 0.00000 |
| 1107 | 110 | GLU | H | -36.01498 | -36.01786 | 105.00992 | B1 | 28 | 0.00000 |
| 1108 | 110 | GLU | CA | -36.20315 | -33.92985 | 105.08184 | B1 | 28 | 0.00000 |
| 1109 | 110 | GLU | CB | -35.80977 | -33.47627 | 106.49578 | B1 | 28 | 0.00000 |
| 1110 | 110 | GLU | CG | -35.32216 | -32.02210 | 106.60993 | B1 | 28 | 0.00000 |
| 1111 | 110 | GLU | CD | -33.83808 | -31.87178 | 106.30413 | B1 | 28 | 0.00000 |
| 1112 | 110 | GLU | OE1 | -33.37957 | -30.74951 | 106.10521 | B1 | 28 | 0.00000 |
| 1113 | 110 | GLU | OE2 | -33.09671 | -32.85201 | 106.36491 | B1 | 28 | 0.00000 |
| 1114 | 110 | GLU | C | -35.01026 | -33.94076 | 104.15500 | B1 | 28 | 0.00000 |
| 1115 | 110 | GLU | O | -34.25577 | -34.90807 | 104.11585 | B1 | 28 | 0.00000 |
| 1116 | 111 | ARG | N | -34.89439 | -32.86843 | 103.37222 | B1 | 29 | 0.00000 |
| 1117 | 111 | ARG | H | -35.61365 | -32.16766 | 103.37387 | B1 | 29 | 0.00000 |
| 1118 | 111 | ARG | CA | -33.75645 | -32.74903 | 102.46249 | B1 | 29 | 0.00000 |
| 1119 | 111 | ARG | CB | -33.99004 | -33.60407 | 101.20352 | B1 | 29 | 0.00000 |
| 1120 | 111 | ARG | CG | -35.45106 | -33.70037 | 100.75305 | B1 | 29 | 0.00000 |
| 1121 | 111 | ARG | CD | -35.67880 | -34.83036 | 99.75174 | B1 | 29 | 0.00000 |
| 1122 | 111 | ARG | NE | -37.09124 | -35.21147 | 99.72614 | B1 | 29 | 0.00000 |
| 1123 | 111 | ARG | HE | -37.71860 | -34.61357 | 100.22757 | B1 | 29 | 0.00000 |
| 1124 | 111 | ARG | CZ | -37.50098 | -36.32384 | 99.09789 | B1 | 29 | 0.00000 |
| 1125 | 111 | ARG | NH1 | -38.78116 | -36.68971 | 99.16119 | B1 | 29 | 0.00000 |
| 1126 | 111 | ARG | HH11 | -39.12269 | -37.49888 | 98.68276 | B1 | 29 | 0.00000 |
| 1127 | 111 | ARG | HH12 | -39.43712 | -36.16699 | 99.70940 | B1 | 29 | 0.00000 |
| 1128 | 111 | ARG | NH2 | -36.63391 | -37.06893 | 98.41518 | B1 | 29 | 0.00000 |
| 1129 | 111 | ARG | HH21 | -36.91501 | -37.90348 | 97.94325 | B1 | 29 | 0.00000 |
| 1130 | 111 | ARG | HH22 | -35.67503 | -36.78688 | 98.36264 | B1 | 29 | 0.00000 |
| 1131 | 111 | ARG | C | -33.49135 | -31.31194 | 102.08170 | B1 | 29 | 0.00000 |
| 1132 | 111 | ARG | O | -34.39395 | -30.54569 | 101.76699 | B1 | 29 | 0.00000 |
| 1133 | 112 | CYS | N | -32.20568 | -30.97057 | 102.12414 | B1 | 30 | 0.00000 |
| 1134 | 112 | CYS | H | -31.50733 | -31.64380 | 102.37455 | B1 | 30 | 0.00000 |
| 1135 | 112 | CYS | CA | -31.80468 | -29.62360 | 101.73826 | B1 | 30 | 0.00000 |
| 1136 | 112 | CYS | CB | -31.12874 | -28.92365 | 102.91930 | B1 | 30 | 0.00000 |
| 1137 | 112 | CYS | SG | -30.70297 | -27.19555 | 102.57697 | B1 | 30 | 0.00000 |
| 1138 | 112 | CYS | C | -30.87388 | -29.64998 | 100.54380 | B1 | 30 | 0.00000 |
| 1139 | 112 | CYS | O | -29.97769 | -30.48052 | 100.40406 | B1 | 30 | 0.00000 |
| 1140 | 113 | ILE | N | -31.15975 | -28.70696 | 99.65078 | B1 | 31 | 0.00000 |
| 1141 | 113 | ILE | H | -31.84193 | -28.00116 | 99.86111 | B1 | 31 | 0.00000 |
| 1142 | 113 | ILE | CA | -30.55306 | -28.70228 | 98.32464 | B1 | 31 | 0.00000 |
| 1143 | 113 | ILE | CB | -31.56021 | -29.33526 | 97.30706 | B1 | 31 | 0.00000 |
| 1144 | 113 | ILE | CG2 | -33.00339 | -29.37434 | 97.82323 | B1 | 31 | 0.00000 |
| 1145 | 113 | ILE | CG1 | -31.52431 | -28.74184 | 95.89635 | B1 | 31 | 0.00000 |
| 1146 | 113 | ILE | CD | -32.44047 | -29.50025 | 94.93272 | B1 | 31 | 0.00000 |
| 1147 | 113 | ILE | C | -30.08576 | -27.29665 | 97.96536 | B1 | 31 | 0.00000 |
| 1148 | 113 | ILE | O | -30.75333 | -26.29900 | 98.21317 | B1 | 31 | 0.00000 |

FIG. 19

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1149 | 114 | TYR | N | 28.87010 | -27.25564 | 97.41665 | B1 | 32 | 0.00000 |
| 1150 | 114 | TYR | H | -28.42970 | -28.10151 | 97.10297 | B1 | 32 | 0.00000 |
| 1151 | 114 | TYR | CA | -28.22036 | -25.98264 | 97.11462 | B1 | 32 | 0.00000 |
| 1152 | 114 | TYR | CB | -26.80088 | -26.01933 | 97.71345 | B1 | 32 | 0.00000 |
| 1153 | 114 | TYR | CG | -26.01127 | -24.72107 | 97.61311 | B1 | 32 | 0.00000 |
| 1154 | 114 | TYR | CD1 | -26.62770 | -23.45825 | 97.79068 | B1 | 32 | 0.00000 |
| 1155 | 114 | TYR | CE1 | -25.84886 | -22.28083 | 97.75267 | B1 | 32 | 0.00000 |
| 1156 | 114 | TYR | CD2 | -24.61824 | -24.80211 | 97.38751 | B1 | 32 | 0.00000 |
| 1157 | 114 | TYR | CE2 | -23.83841 | -23.62651 | 97.34588 | B1 | 32 | 0.00000 |
| 1158 | 114 | TYR | CZ | -24.45600 | -22.36940 | 97.53154 | B1 | 32 | 0.00000 |
| 1159 | 114 | TYR | OH | -23.68967 | -21.21917 | 97.50979 | B1 | 32 | 0.00000 |
| 1160 | 114 | TYR | HH | -22.79676 | -21.43015 | 97.21984 | B1 | 32 | 0.00000 |
| 1161 | 114 | TYR | C | -28.14723 | -25.83215 | 95.61430 | B1 | 32 | 0.00000 |
| 1162 | 114 | TYR | O | -27.66375 | -26.70965 | 94.91236 | B1 | 32 | 0.00000 |
| 1163 | 115 | ASN | N | -28.66823 | -24.69995 | 95.12919 | B1 | 33 | 0.00000 |
| 1164 | 115 | ASN | H | -29.03092 | -24.02391 | 95.77643 | B1 | 33 | 0.00000 |
| 1165 | 115 | ASN | CA | -28.63762 | -24.41545 | 93.68566 | B1 | 33 | 0.00000 |
| 1166 | 115 | ASN | CB | -27.27049 | -23.84385 | 93.27078 | B1 | 33 | 0.00000 |
| 1167 | 115 | ASN | CG | -27.00239 | -22.43118 | 93.78440 | B1 | 33 | 0.00000 |
| 1168 | 115 | ASN | OD1 | -26.55389 | -22.16954 | 94.85370 | B1 | 33 | 0.00000 |
| 1169 | 115 | ASN | ND2 | -27.51765 | -21.48359 | 92.96271 | B1 | 33 | 0.00000 |
| 1170 | 115 | ASN | HD21 | -28.04883 | -21.70692 | 92.14797 | B1 | 33 | 0.00000 |
| 1171 | 115 | ASN | HD22 | -27.29503 | -20.52370 | 93.13946 | B1 | 33 | 0.00000 |
| 1172 | 115 | ASN | C | -28.96318 | -25.59300 | 92.77321 | B1 | 33 | 0.00000 |
| 1173 | 115 | ASN | O | -28.22150 | -25.91402 | 91.85250 | B1 | 33 | 0.00000 |
| 1174 | 116 | GLN | N | -30.10691 | -26.23583 | 93.07767 | B1 | 34 | 0.00000 |
| 1175 | 116 | GLN | H | -30.66790 | -25.92614 | 93.84830 | B1 | 34 | 0.00000 |
| 1176 | 116 | GLN | CA | -30.60575 | -27.38897 | 92.31212 | B1 | 34 | 0.00000 |
| 1177 | 116 | GLN | CB | -30.73906 | -26.98635 | 90.82631 | B1 | 34 | 0.00000 |
| 1178 | 116 | GLN | CG | -31.33401 | -27.96419 | 89.80983 | B1 | 34 | 0.00000 |
| 1179 | 116 | GLN | CD | -31.33954 | -27.31473 | 88.43508 | B1 | 34 | 0.00000 |
| 1180 | 116 | GLN | OE1 | -32.32002 | -27.33002 | 87.70605 | B1 | 34 | 0.00000 |
| 1181 | 116 | GLN | NE2 | -30.20428 | -26.71450 | 88.08185 | B1 | 34 | 0.00000 |
| 1182 | 116 | GLN | HE21 | -29.39553 | -26.71396 | 88.67007 | B1 | 34 | 0.00000 |
| 1183 | 116 | GLN | HE22 | -30.15594 | -26.24641 | 87.20205 | B1 | 34 | 0.00000 |
| 1184 | 116 | GLN | C | -29.89899 | -28.73663 | 92.53043 | B1 | 34 | 0.00000 |
| 1185 | 116 | GLN | O | -30.38571 | -29.77893 | 92.10767 | B1 | 34 | 0.00000 |
| 1186 | 117 | GLU | N | -28.76921 | -28.72803 | 93.24838 | B1 | 35 | 0.00000 |
| 1187 | 117 | GLU | H | -28.34990 | -27.88576 | 93.59525 | B1 | 35 | 0.00000 |
| 1188 | 117 | GLU | CA | -28.17324 | -30.02538 | 93.58636 | B1 | 35 | 0.00000 |
| 1189 | 117 | GLU | CB | -26.68237 | -30.02385 | 93.23572 | B1 | 35 | 0.00000 |
| 1190 | 117 | GLU | CG | -26.41125 | -29.71932 | 91.75724 | B1 | 35 | 0.00000 |
| 1191 | 117 | GLU | CD | -24.93459 | -29.87167 | 91.43636 | B1 | 35 | 0.00000 |
| 1192 | 117 | GLU | OE1 | -24.62388 | -30.40776 | 90.37359 | B1 | 35 | 0.00000 |
| 1193 | 117 | GLU | OE2 | -24.09945 | -29.45965 | 92.24135 | B1 | 35 | 0.00000 |
| 1194 | 117 | GLU | C | -28.34342 | -30.39133 | 95.05360 | B1 | 35 | 0.00000 |
| 1195 | 117 | GLU | O | -28.39032 | -29.54087 | 95.93593 | B1 | 35 | 0.00000 |
| 1196 | 118 | GLU | N | -28.45418 | -31.70267 | 95.31151 | B1 | 36 | 0.00000 |
| 1197 | 118 | GLU | H | -28.37884 | -32.37663 | 94.57056 | B1 | 36 | 0.00000 |
| 1198 | 118 | GLU | CA | -28.64640 | -32.12718 | 96.70604 | B1 | 36 | 0.00000 |
| 1199 | 118 | GLU | CB | -28.86529 | -33.64399 | 96.80220 | B1 | 36 | 0.00000 |
| 1200 | 118 | GLU | CG | -30.04821 | -34.25904 | 96.04454 | B1 | 36 | 0.00000 |
| 1201 | 118 | GLU | CD | -30.18685 | -35.73854 | 96.39969 | B1 | 36 | 0.00000 |
| 1202 | 118 | GLU | OE1 | -31.31366 | -36.18552 | 96.62004 | B1 | 36 | 0.00000 |
| 1203 | 118 | GLU | OE2 | -29.17775 | -36.44658 | 96.46236 | B1 | 36 | 0.00000 |
| 1204 | 118 | GLU | C | -27.45968 | -31.79603 | 97.59954 | B1 | 36 | 0.00000 |
| 1205 | 118 | GLU | O | -26.30375 | -31.93771 | 97.22004 | B1 | 36 | 0.00000 |
| 1206 | 119 | SER | N | -27.77719 | -31.35385 | 98.81871 | B1 | 37 | 0.00000 |
| 1207 | 119 | SER | H | -28.73032 | -31.22468 | 99.10568 | B1 | 37 | 0.00000 |
| 1208 | 119 | SER | CA | -26.67523 | -31.09310 | 99.74333 | B1 | 37 | 0.00000 |
| 1209 | 119 | SER | CB | -26.79679 | -29.64425 | 100.25438 | B1 | 37 | 0.00000 |
| 1210 | 119 | SER | OG | -25.62406 | -29.23340 | 100.96654 | B1 | 37 | 0.00000 |
| 1211 | 119 | SER | HG | -25.73840 | -28.33730 | 101.30354 | B1 | 37 | 0.00000 |
| 1212 | 119 | SER | C | -26.64967 | -32.10869 | 100.87899 | B1 | 37 | 0.00000 |

FIG. 20

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1213 | 119 | SER | O | 25.72568 | -32.90554 | 101.03211 | B1 | 37 | 0.00000 |
| 1214 | 120 | VAL | N | -27.72434 | -32.06808 | 101.67561 | B1 | 38 | 0.00000 |
| 1215 | 120 | VAL | H | -28.50026 | -31.45938 | 101.48344 | B1 | 38 | 0.00000 |
| 1216 | 120 | VAL | CA | -27.82678 | -32.99802 | 102.80099 | B1 | 38 | 0.00000 |
| 1217 | 120 | VAL | CB | -27.44790 | -32.32244 | 104.13888 | B1 | 38 | 0.00000 |
| 1218 | 120 | VAL | CG1 | -25.93252 | -32.18078 | 104.29388 | B1 | 38 | 0.00000 |
| 1219 | 120 | VAL | CG2 | -28.15631 | -30.97900 | 104.33500 | B1 | 38 | 0.00000 |
| 1220 | 120 | VAL | C | -29.23777 | -33.53625 | 102.89372 | B1 | 38 | 0.00000 |
| 1221 | 120 | VAL | O | -30.19812 | -32.88656 | 102.49711 | B1 | 38 | 0.00000 |
| 1222 | 121 | ARG | N | -29.34164 | -34.75356 | 103.41944 | B1 | 39 | 0.00000 |
| 1223 | 121 | ARG | H | -28.52525 | -35.27675 | 103.67737 | B1 | 39 | 0.00000 |
| 1224 | 121 | ARG | CA | -30.65941 | -35.37282 | 103.49447 | B1 | 39 | 0.00000 |
| 1225 | 121 | ARG | CB | -30.83879 | -36.26556 | 102.25451 | B1 | 39 | 0.00000 |
| 1226 | 121 | ARG | CG | -32.24891 | -36.83907 | 102.13977 | B1 | 39 | 0.00000 |
| 1227 | 121 | ARG | CD | -32.36448 | -38.11228 | 101.31436 | B1 | 39 | 0.00000 |
| 1228 | 121 | ARG | NE | -33.46636 | -38.89614 | 101.86585 | B1 | 39 | 0.00000 |
| 1229 | 121 | ARG | HE | -33.58314 | -38.82444 | 102.86363 | B1 | 39 | 0.00000 |
| 1230 | 121 | ARG | CZ | -34.21779 | -39.71705 | 101.13259 | B1 | 39 | 0.00000 |
| 1231 | 121 | ARG | NH1 | -35.18842 | -40.40193 | 101.73316 | B1 | 39 | 0.00000 |
| 1232 | 121 | ARG | HH11 | -35.77971 | -41.03741 | 101.23780 | B1 | 39 | 0.00000 |
| 1233 | 121 | ARG | HH12 | -35.33365 | -40.28453 | 102.71808 | B1 | 39 | 0.00000 |
| 1234 | 121 | ARG | NH2 | -33.99786 | -39.84536 | 99.82444 | B1 | 39 | 0.00000 |
| 1235 | 121 | ARG | HH21 | -34.53079 | -40.47140 | 99.25675 | B1 | 39 | 0.00000 |
| 1236 | 121 | ARG | HH22 | -33.27054 | -39.30635 | 99.39731 | B1 | 39 | 0.00000 |
| 1237 | 121 | ARG | C | -30.80743 | -36.21013 | 104.75602 | B1 | 39 | 0.00000 |
| 1238 | 121 | ARG | O | -29.86515 | -36.82872 | 105.23483 | B1 | 39 | 0.00000 |
| 1239 | 122 | PHE | N | -32.04075 | -36.24095 | 105.26404 | B1 | 40 | 0.00000 |
| 1240 | 122 | PHE | H | -32.75061 | -35.63810 | 104.89111 | B1 | 40 | 0.00000 |
| 1241 | 122 | PHE | CA | -32.40668 | -37.26064 | 106.24769 | B1 | 40 | 0.00000 |
| 1242 | 122 | PHE | CB | -33.75724 | -36.87165 | 106.85296 | B1 | 40 | 0.00000 |
| 1243 | 122 | PHE | CG | -33.64992 | -36.46831 | 108.30418 | B1 | 40 | 0.00000 |
| 1244 | 122 | PHE | CD1 | -32.56100 | -35.69712 | 108.77664 | B1 | 40 | 0.00000 |
| 1245 | 122 | PHE | CD2 | -34.66985 | -36.87929 | 109.19094 | B1 | 40 | 0.00000 |
| 1246 | 122 | PHE | CE1 | -32.49275 | -35.34303 | 110.14035 | B1 | 40 | 0.00000 |
| 1247 | 122 | PHE | CE2 | -34.60187 | -36.52254 | 110.55431 | B1 | 40 | 0.00000 |
| 1248 | 122 | PHE | CZ | -33.51285 | -35.75823 | 111.02379 | B1 | 40 | 0.00000 |
| 1249 | 122 | PHE | C | -32.57844 | -38.62424 | 105.60697 | B1 | 40 | 0.00000 |
| 1250 | 122 | PHE | O | -33.34168 | -38.79208 | 104.65587 | B1 | 40 | 0.00000 |
| 1251 | 123 | ASP | N | -31.06201 | -39.60796 | 106.15389 | B1 | 41 | 0.00000 |
| 1252 | 123 | ASP | H | -31.23184 | -39.47015 | 106.92548 | B1 | 41 | 0.00000 |
| 1253 | 123 | ASP | CA | -32.08552 | -40.93522 | 105.58825 | B1 | 41 | 0.00000 |
| 1254 | 123 | ASP | CB | -30.85171 | -41.81726 | 105.76445 | B1 | 41 | 0.00000 |
| 1255 | 123 | ASP | CG | -29.93161 | -41.56041 | 104.59405 | B1 | 41 | 0.00000 |
| 1256 | 123 | ASP | OD1 | -28.81173 | -41.11310 | 104.81757 | B1 | 41 | 0.00000 |
| 1257 | 123 | ASP | OD2 | -30.34905 | -41.80191 | 103.45856 | B1 | 41 | 0.00000 |
| 1258 | 123 | ASP | C | -33.32362 | -41.63618 | 106.09965 | B1 | 41 | 0.00000 |
| 1259 | 123 | ASP | O | -34.00966 | -41.21121 | 107.02319 | B1 | 41 | 0.00000 |
| 1260 | 124 | SER | N | -33.62443 | -42.74250 | 105.41429 | B1 | 42 | 0.00000 |
| 1261 | 124 | SER | H | -32.95329 | -43.10971 | 104.76900 | B1 | 42 | 0.00000 |
| 1262 | 124 | SER | CA | -34.94425 | -43.35498 | 105.58880 | B1 | 42 | 0.00000 |
| 1263 | 124 | SER | CB | -35.18779 | -44.37028 | 104.46149 | B1 | 42 | 0.00000 |
| 1264 | 124 | SER | OG | -36.57945 | -44.70776 | 104.37671 | B1 | 42 | 0.00000 |
| 1265 | 124 | SER | HG | -36.91089 | -44.87590 | 105.27413 | B1 | 42 | 0.00000 |
| 1266 | 124 | SER | C | -35.21640 | -44.01057 | 106.93634 | B1 | 42 | 0.00000 |
| 1267 | 124 | SER | O | -36.33538 | -44.42223 | 107.22372 | B1 | 42 | 0.00000 |
| 1268 | 125 | ASP | N | -34.16447 | -44.10325 | 107.74330 | B1 | 43 | 0.00000 |
| 1269 | 125 | ASP | H | -33.26228 | -43.73425 | 107.50494 | B1 | 43 | 0.00000 |
| 1270 | 125 | ASP | CA | -34.30492 | -44.60689 | 109.10471 | B1 | 43 | 0.00000 |
| 1271 | 125 | ASP | CB | -32.96210 | -45.24580 | 109.50620 | B1 | 43 | 0.00000 |
| 1272 | 125 | ASP | CG | -31.82155 | -44.23245 | 109.55779 | B1 | 43 | 0.00000 |
| 1273 | 125 | ASP | OD1 | -31.89194 | -43.19553 | 108.89075 | B1 | 43 | 0.00000 |
| 1274 | 125 | ASP | OD2 | -30.87249 | -44.45676 | 110.29614 | B1 | 43 | 0.00000 |
| 1275 | 125 | ASP | C | -34.69374 | -43.52244 | 110.10428 | B1 | 43 | 0.00000 |
| 1276 | 125 | ASP | O | -35.10540 | -43.78441 | 111.22872 | B1 | 43 | 0.00000 |

FIG. 21

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1277 | 126 | VAL | N | - .51615 | -42.26751 | 109.64790 | B1 | 44 | 0.00000 |
| 1278 | 126 | VAL | H | -34.20939 | -42.12308 | 108.70456 | B1 | 44 | 0.00000 |
| 1279 | 126 | VAL | CA | -34.59346 | -41.07914 | 110.50496 | B1 | 44 | 0.00000 |
| 1280 | 126 | VAL | CB | -36.04814 | -40.82462 | 110.97592 | B1 | 44 | 0.00000 |
| 1281 | 126 | VAL | CG1 | -36.22164 | -39.41758 | 111.54094 | B1 | 44 | 0.00000 |
| 1282 | 126 | VAL | CG2 | -37.04494 | -41.00281 | 109.82481 | B1 | 44 | 0.00000 |
| 1283 | 126 | VAL | C | -33.57625 | -41.13739 | 111.64961 | B1 | 44 | 0.00000 |
| 1284 | 126 | VAL | O | -33.78819 | -40.75401 | 112.79533 | B1 | 44 | 0.00000 |
| 1285 | 127 | GLY | N | -32.41541 | -41.66443 | 111.25324 | B1 | 45 | 0.00000 |
| 1286 | 127 | GLY | H | -32.31598 | -42.01122 | 110.31755 | B1 | 45 | 0.00000 |
| 1287 | 127 | GLY | CA | -31.32244 | -41.88201 | 112.19529 | B1 | 45 | 0.00000 |
| 1288 | 127 | GLY | C | -29.94594 | -41.56889 | 111.62542 | B1 | 45 | 0.00000 |
| 1289 | 127 | GLY | O | -29.03055 | -41.21776 | 112.35962 | B1 | 45 | 0.00000 |
| 1290 | 128 | GLU | N | -29.81143 | -41.65704 | 110.29545 | B1 | 46 | 0.00000 |
| 1291 | 128 | GLU | H | -30.48653 | -42.13586 | 109.72534 | B1 | 46 | 0.00000 |
| 1292 | 128 | GLU | CA | -28.56256 | -41.14297 | 109.73120 | B1 | 46 | 0.00000 |
| 1293 | 128 | GLU | CB | -27.75197 | -42.29481 | 109.11709 | B1 | 46 | 0.00000 |
| 1294 | 128 | GLU | CG | -26.29316 | -42.25781 | 109.59860 | B1 | 46 | 0.00000 |
| 1295 | 128 | GLU | CD | -25.44181 | -43.28422 | 108.87693 | B1 | 46 | 0.00000 |
| 1296 | 128 | GLU | OE1 | -24.49646 | -42.88073 | 108.19992 | B1 | 46 | 0.00000 |
| 1297 | 128 | GLU | OE2 | -25.71010 | -44.47773 | 109.00348 | B1 | 46 | 0.00000 |
| 1298 | 128 | GLU | C | -28.71376 | -39.98012 | 108.75031 | B1 | 46 | 0.00000 |
| 1299 | 128 | GLU | O | -29.80604 | -39.57375 | 108.35724 | B1 | 46 | 0.00000 |
| 1300 | 129 | TYR | N | -27.54735 | -39.42619 | 108.38931 | B1 | 47 | 0.00000 |
| 1301 | 129 | TYR | H | -26.68498 | -39.83420 | 108.68820 | B1 | 47 | 0.00000 |
| 1302 | 129 | TYR | CA | -27.50019 | -38.29454 | 107.46434 | B1 | 47 | 0.00000 |
| 1303 | 129 | TYR | CB | -26.63842 | -37.15326 | 108.01560 | B1 | 47 | 0.00000 |
| 1304 | 129 | TYR | CG | -27.30857 | -36.34222 | 109.09443 | B1 | 47 | 0.00000 |
| 1305 | 129 | TYR | CD1 | -26.67181 | -36.21958 | 110.34811 | B1 | 47 | 0.00000 |
| 1306 | 129 | TYR | CE1 | -27.25566 | -35.42131 | 111.35148 | B1 | 47 | 0.00000 |
| 1307 | 129 | TYR | CD2 | -28.52827 | -35.67832 | 108.83210 | B1 | 47 | 0.00000 |
| 1308 | 129 | TYR | CE2 | -29.11235 | -34.88063 | 109.83571 | B1 | 47 | 0.00000 |
| 1309 | 129 | TYR | CZ | -28.47327 | -34.75726 | 111.08860 | B1 | 47 | 0.00000 |
| 1310 | 129 | TYR | OH | -29.05005 | -33.98459 | 112.07221 | B1 | 47 | 0.00000 |
| 1311 | 129 | TYR | HH | -29.70394 | -33.40059 | 111.67732 | B1 | 47 | 0.00000 |
| 1312 | 129 | TYR | C | -26.82531 | -38.64384 | 106.15941 | B1 | 47 | 0.00000 |
| 1313 | 129 | TYR | O | -25.66697 | -39.04407 | 106.10492 | B1 | 47 | 0.00000 |
| 1314 | 130 | ARG | N | -27.55686 | -38.38162 | 105.08581 | B1 | 48 | 0.00000 |
| 1315 | 130 | ARG | H | -28.51666 | -38.10451 | 105.16735 | B1 | 48 | 0.00000 |
| 1316 | 130 | ARG | CA | -26.87326 | -38.41254 | 103.80227 | B1 | 48 | 0.00000 |
| 1317 | 130 | ARG | CB | -27.85650 | -38.84699 | 102.71647 | B1 | 48 | 0.00000 |
| 1318 | 130 | ARG | CG | -27.21143 | -39.00526 | 101.34112 | B1 | 48 | 0.00000 |
| 1319 | 130 | ARG | CD | -28.23975 | -39.41974 | 100.29808 | B1 | 48 | 0.00000 |
| 1320 | 130 | ARG | NE | -27.66322 | -39.38333 | 98.95629 | B1 | 48 | 0.00000 |
| 1321 | 130 | ARG | HE | -26.82589 | -38.85034 | 98.82833 | B1 | 48 | 0.00000 |
| 1322 | 130 | ARG | CZ | -28.29934 | -39.96348 | 97.93202 | B1 | 48 | 0.00000 |
| 1323 | 130 | ARG | NH1 | -27.82365 | -39.81313 | 96.69917 | B1 | 48 | 0.00000 |
| 1324 | 130 | ARG | HH11 | -28.26738 | -40.23513 | 95.90996 | B1 | 48 | 0.00000 |
| 1325 | 130 | ARG | HH12 | -27.01064 | -39.25297 | 96.53955 | B1 | 48 | 0.00000 |
| 1326 | 130 | ARG | NH2 | -29.39843 | -40.68730 | 98.14392 | B1 | 48 | 0.00000 |
| 1327 | 130 | ARG | HH21 | -29.90446 | -41.10492 | 97.39118 | B1 | 48 | 0.00000 |
| 1328 | 130 | ARG | HH22 | -29.72741 | -40.81930 | 99.07957 | B1 | 48 | 0.00000 |
| 1329 | 130 | ARG | C | -26.28084 | -37.06053 | 103.45986 | B1 | 48 | 0.00000 |
| 1330 | 130 | ARG | O | -26.96293 | -36.11772 | 103.07688 | B1 | 48 | 0.00000 |
| 1331 | 131 | ALA | N | -24.95816 | -36.99899 | 103.58668 | B1 | 49 | 0.00000 |
| 1332 | 131 | ALA | H | -24.45069 | -37.77908 | 103.95192 | B1 | 49 | 0.00000 |
| 1333 | 131 | ALA | CA | -24.28607 | -35.84094 | 102.98902 | B1 | 49 | 0.00000 |
| 1334 | 131 | ALA | CB | -23.06137 | -35.44271 | 103.80801 | B1 | 49 | 0.00000 |
| 1335 | 131 | ALA | C | -23.85084 | -36.20833 | 101.58658 | B1 | 49 | 0.00000 |
| 1336 | 131 | ALA | O | -23.17892 | -37.20532 | 101.36065 | B1 | 49 | 0.00000 |
| 1337 | 132 | VAL | N | -24.28495 | -35.38774 | 100.63154 | B1 | 50 | 0.00000 |
| 1338 | 132 | VAL | H | -24.78984 | -34.54695 | 100.85567 | B1 | 50 | 0.00000 |
| 1339 | 132 | VAL | CA | -24.05930 | -35.79619 | 99.24192 | B1 | 50 | 0.00000 |
| 1340 | 132 | VAL | CB | -25.12578 | -35.11200 | 98.36560 | B1 | 50 | 0.00000 |

FIG. 22

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1341 | 132 | VAL | CG1 | 5.02505 | -35.45687 | 96.87606 | B1 | 50 | 0.00000 |
| 1342 | 132 | VAL | CG2 | -26.51048 | -35.48893 | 98.89777 | B1 | 50 | 0.00000 |
| 1343 | 132 | VAL | C | -22.64446 | -35.53393 | 98.73419 | B1 | 50 | 0.00000 |
| 1344 | 132 | VAL | O | -22.12598 | -36.19257 | 97.84114 | B1 | 50 | 0.00000 |
| 1345 | 133 | THR | N | -22.01646 | -34.53567 | 99.35299 | B1 | 51 | 0.00000 |
| 1346 | 133 | THR | H | -22.44036 | -34.04272 | 100.11190 | B1 | 51 | 0.00000 |
| 1347 | 133 | THR | CA | -20.68297 | -34.13851 | 98.91128 | B1 | 51 | 0.00000 |
| 1348 | 133 | THR | CB | -20.84979 | -33.09962 | 97.76600 | B1 | 51 | 0.00000 |
| 1349 | 133 | THR | OG1 | -19.58519 | -32.56706 | 97.34397 | B1 | 51 | 0.00000 |
| 1350 | 133 | THR | HG1 | -19.69018 | -32.10136 | 96.50551 | B1 | 51 | 0.00000 |
| 1351 | 133 | THR | CG2 | -21.81730 | -31.96947 | 98.12788 | B1 | 51 | 0.00000 |
| 1352 | 133 | THR | C | -19.91735 | -33.59750 | 100.10846 | B1 | 51 | 0.00000 |
| 1353 | 133 | THR | O | -20.48697 | -33.30952 | 101.15881 | B1 | 51 | 0.00000 |
| 1354 | 134 | GLU | N | -18.60119 | -33.44216 | 99.91793 | B1 | 52 | 0.00000 |
| 1355 | 134 | GLU | H | -18.20352 | -33.65725 | 99.02398 | B1 | 52 | 0.00000 |
| 1356 | 134 | GLU | CA | -17.75238 | -32.88738 | 100.97647 | B1 | 52 | 0.00000 |
| 1357 | 134 | GLU | CB | -16.30452 | -32.81284 | 100.49482 | B1 | 52 | 0.00000 |
| 1358 | 134 | GLU | CG | -15.76229 | -34.17073 | 100.03844 | B1 | 52 | 0.00000 |
| 1359 | 134 | GLU | CD | -14.31377 | -34.04410 | 99.60488 | B1 | 52 | 0.00000 |
| 1360 | 134 | GLU | OE1 | -13.54341 | -34.96158 | 99.88007 | B1 | 52 | 0.00000 |
| 1361 | 134 | GLU | OE2 | -13.96021 | -33.03519 | 98.99487 | B1 | 52 | 0.00000 |
| 1362 | 134 | GLU | C | -18.18601 | -31.51310 | 101.45728 | B1 | 52 | 0.00000 |
| 1363 | 134 | GLU | O | -17.97884 | -31.11916 | 102.59352 | B1 | 52 | 0.00000 |
| 1364 | 135 | LEU | N | -18.87611 | -30.80674 | 100.55812 | B1 | 53 | 0.00000 |
| 1365 | 135 | LEU | H | -18.92762 | -31.13340 | 99.61398 | B1 | 53 | 0.00000 |
| 1366 | 135 | LEU | CA | -19.55727 | -29.57029 | 100.94931 | B1 | 53 | 0.00000 |
| 1367 | 135 | LEU | CB | -20.29914 | -29.06218 | 99.70959 | B1 | 53 | 0.00000 |
| 1368 | 135 | LEU | CG | -20.12211 | -27.57937 | 99.38843 | B1 | 53 | 0.00000 |
| 1369 | 135 | LEU | CD1 | -20.93390 | -26.68772 | 100.32666 | B1 | 53 | 0.00000 |
| 1370 | 135 | LEU | CD2 | -18.63204 | -27.23870 | 99.36436 | B1 | 53 | 0.00000 |
| 1371 | 135 | LEU | C | -20.53099 | -29.72915 | 102.11412 | B1 | 53 | 0.00000 |
| 1372 | 135 | LEU | O | -20.60025 | -28.93514 | 103.04463 | B1 | 53 | 0.00000 |
| 1373 | 136 | GLY | N | -21.29082 | -30.82221 | 102.02891 | B1 | 54 | 0.00000 |
| 1374 | 136 | GLY | H | -21.14062 | -31.49656 | 101.30480 | B1 | 54 | 0.00000 |
| 1375 | 136 | GLY | CA | -22.25373 | -31.10000 | 103.08935 | B1 | 54 | 0.00000 |
| 1376 | 136 | GLY | C | -21.66227 | -31.85099 | 104.26834 | B1 | 54 | 0.00000 |
| 1377 | 136 | GLY | O | -22.17280 | -31.82013 | 105.38053 | B1 | 54 | 0.00000 |
| 1378 | 137 | ARG | N | -20.54192 | -32.53644 | 104.01306 | B1 | 55 | 0.00000 |
| 1379 | 137 | ARG | H | -20.17033 | -32.57514 | 103.08296 | B1 | 55 | 0.00000 |
| 1380 | 137 | ARG | CA | -19.94165 | -33.32437 | 105.09532 | B1 | 55 | 0.00000 |
| 1381 | 137 | ARG | CB | -18.67070 | -34.02762 | 104.58318 | B1 | 55 | 0.00000 |
| 1382 | 137 | ARG | CG | -18.13008 | -35.07893 | 105.55025 | B1 | 55 | 0.00000 |
| 1383 | 137 | ARG | CD | -19.16855 | -36.15719 | 105.85371 | B1 | 55 | 0.00000 |
| 1384 | 137 | ARG | NE | -18.66781 | -37.06640 | 106.87657 | B1 | 55 | 0.00000 |
| 1385 | 137 | ARG | HE | -17.93002 | -36.71980 | 107.47204 | B1 | 55 | 0.00000 |
| 1386 | 137 | ARG | CZ | -19.21896 | -38.26612 | 107.07086 | B1 | 55 | 0.00000 |
| 1387 | 137 | ARG | NH1 | -18.67934 | -39.07643 | 107.97489 | B1 | 55 | 0.00000 |
| 1388 | 137 | ARG | HH11 | -19.03969 | -39.99255 | 108.14749 | B1 | 55 | 0.00000 |
| 1389 | 137 | ARG | HH12 | -17.88763 | -38.75541 | 108.49972 | B1 | 55 | 0.00000 |
| 1390 | 137 | ARG | NH2 | -20.29085 | -38.64369 | 106.37214 | B1 | 55 | 0.00000 |
| 1391 | 137 | ARG | HH21 | -20.72192 | -39.53705 | 106.49834 | B1 | 55 | 0.00000 |
| 1392 | 137 | ARG | HH22 | -20.68879 | -38.01490 | 105.70437 | B1 | 55 | 0.00000 |
| 1393 | 137 | ARG | C | -19.76330 | -32.65026 | 106.46929 | B1 | 55 | 0.00000 |
| 1394 | 137 | ARG | O | -20.33202 | -33.13638 | 107.44172 | B1 | 55 | 0.00000 |
| 1395 | 138 | PRO | N | -19.03095 | -31.51331 | 106.56277 | B1 | 56 | 0.00000 |
| 1396 | 138 | PRO | CD | -18.26903 | -30.78028 | 105.55482 | B1 | 56 | 0.00000 |
| 1397 | 138 | PRO | CA | -18.92500 | -30.86885 | 107.87839 | B1 | 56 | 0.00000 |
| 1398 | 138 | PRO | CB | -18.00966 | -29.66775 | 107.61418 | B1 | 56 | 0.00000 |
| 1399 | 138 | PRO | CG | -17.22921 | -30.01427 | 106.35389 | B1 | 56 | 0.00000 |
| 1400 | 138 | PRO | C | -20.24853 | -30.39451 | 108.45452 | B1 | 56 | 0.00000 |
| 1401 | 138 | PRO | O | -20.38873 | -30.20105 | 109.65243 | B1 | 56 | 0.00000 |
| 1402 | 139 | ASP | N | -21.22822 | -30.19487 | 107.56513 | B1 | 57 | 0.00000 |
| 1403 | 139 | ASP | H | -21.12955 | -30.45258 | 106.60296 | B1 | 57 | 0.00000 |
| 1404 | 139 | ASP | CA | -22.54445 | -29.76374 | 108.02635 | B1 | 57 | 0.00000 |

FIG. 23

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1405 | 139 | ASP | CB | 3.29481 | -29.22794 | 106.80729 | B1 | 57 | 0.00000 |
| 1406 | 139 | ASP | CG | -24.50680 | -28.44150 | 107.23406 | B1 | 57 | 0.00000 |
| 1407 | 139 | ASP | OD1 | -24.33925 | -27.25955 | 107.53698 | B1 | 57 | 0.00000 |
| 1408 | 139 | ASP | OD2 | -25.59590 | -29.00937 | 107.24891 | B1 | 57 | 0.00000 |
| 1409 | 139 | ASP | C | -23.29009 | -30.90651 | 108.70646 | B1 | 57 | 0.00000 |
| 1410 | 139 | ASP | O | -23.84428 | -30.79944 | 109.79628 | B1 | 57 | 0.00000 |
| 1411 | 140 | ALA | N | -23.18867 | -32.06950 | 108.04975 | B1 | 58 | 0.00000 |
| 1412 | 140 | ALA | H | -22.77745 | -32.09325 | 107.13514 | B1 | 58 | 0.00000 |
| 1413 | 140 | ALA | CA | -23.64141 | -33.29863 | 108.70194 | B1 | 58 | 0.00000 |
| 1414 | 140 | ALA | CB | -23.39932 | -34.51285 | 107.80148 | B1 | 58 | 0.00000 |
| 1415 | 140 | ALA | C | -22.96994 | -33.52591 | 110.04660 | B1 | 58 | 0.00000 |
| 1416 | 140 | ALA | O | -23.61501 | -33.62460 | 111.08086 | B1 | 58 | 0.00000 |
| 1417 | 141 | GLU | N | -21.63141 | -33.53710 | 110.01537 | B1 | 59 | 0.00000 |
| 1418 | 141 | GLU | H | -21.14260 | -33.44422 | 109.14251 | B1 | 59 | 0.00000 |
| 1419 | 141 | GLU | CA | -20.88131 | -33.73045 | 111.26272 | B1 | 59 | 0.00000 |
| 1420 | 141 | GLU | CB | -19.38545 | -33.75474 | 110.92637 | B1 | 59 | 0.00000 |
| 1421 | 141 | GLU | CG | -19.08157 | -34.92155 | 109.97183 | B1 | 59 | 0.00000 |
| 1422 | 141 | GLU | CD | -17.65605 | -34.91070 | 109.44677 | B1 | 59 | 0.00000 |
| 1423 | 141 | GLU | OE1 | -17.21662 | -35.95752 | 108.96182 | B1 | 59 | 0.00000 |
| 1424 | 141 | GLU | OE2 | -16.99658 | -33.87375 | 109.50288 | B1 | 59 | 0.00000 |
| 1425 | 141 | GLU | C | -21.20315 | -32.72395 | 112.36696 | B1 | 59 | 0.00000 |
| 1426 | 141 | GLU | O | -21.35204 | -33.05368 | 113.53869 | B1 | 59 | 0.00000 |
| 1427 | 142 | TYR | N | -21.39109 | -31.47026 | 111.93865 | B1 | 60 | 0.00000 |
| 1428 | 142 | TYR | H | -21.16858 | -31.22939 | 110.99159 | B1 | 60 | 0.00000 |
| 1429 | 142 | TYR | CA | -21.91640 | -30.42572 | 112.82625 | B1 | 60 | 0.00000 |
| 1430 | 142 | TYR | CB | -22.17510 | -29.18770 | 111.95478 | B1 | 60 | 0.00000 |
| 1431 | 142 | TYR | CG | -22.15441 | -27.86866 | 112.68902 | B1 | 60 | 0.00000 |
| 1432 | 142 | TYR | CD1 | -20.91930 | -27.21121 | 112.08286 | B1 | 60 | 0.00000 |
| 1433 | 142 | TYR | CE1 | -20.89216 | -25.94177 | 113.49633 | B1 | 60 | 0.00000 |
| 1434 | 142 | TYR | CD2 | -23.36373 | -27.27306 | 113.11310 | B1 | 60 | 0.00000 |
| 1435 | 142 | TYR | CE2 | -23.33600 | -26.00211 | 113.72688 | B1 | 60 | 0.00000 |
| 1436 | 142 | TYR | CZ | -22.10013 | -25.34007 | 113.91274 | B1 | 60 | 0.00000 |
| 1437 | 142 | TYR | OH | -22.06472 | -24.08718 | 114.49226 | B1 | 60 | 0.00000 |
| 1438 | 142 | TYR | HH | -22.95958 | -23.75980 | 114.62492 | B1 | 60 | 0.00000 |
| 1439 | 142 | TYR | C | -23.20365 | -30.84932 | 113.52485 | B1 | 60 | 0.00000 |
| 1440 | 142 | TYR | O | -23.33185 | -30.86335 | 114.74427 | B1 | 60 | 0.00000 |
| 1441 | 143 | TRP | N | -24.16819 | -31.24530 | 112.69102 | B1 | 61 | 0.00000 |
| 1442 | 143 | TRP | H | -24.01203 | -31.27353 | 111.69669 | B1 | 61 | 0.00000 |
| 1443 | 143 | TRP | CA | -25.46084 | -31.65772 | 113.24427 | B1 | 61 | 0.00000 |
| 1444 | 143 | TRP | CB | -26.46502 | -31.82534 | 112.10045 | B1 | 61 | 0.00000 |
| 1445 | 143 | TRP | CG | -26.82927 | -30.51319 | 111.43167 | B1 | 61 | 0.00000 |
| 1446 | 143 | TRP | CD2 | -27.59514 | -30.35383 | 110.26190 | B1 | 61 | 0.00000 |
| 1447 | 143 | TRP | CE2 | -27.68725 | -28.88192 | 110.01923 | B1 | 61 | 0.00000 |
| 1448 | 143 | TRP | CE3 | -28.23171 | -31.24445 | 109.37526 | B1 | 61 | 0.00000 |
| 1449 | 143 | TRP | CD1 | -26.49404 | -29.20408 | 111.84528 | B1 | 61 | 0.00000 |
| 1450 | 143 | TRP | NE1 | -26.99373 | -28.24161 | 111.01939 | B1 | 61 | 0.00000 |
| 1451 | 143 | TRP | HE1 | -26.86335 | -27.27405 | 111.09738 | B1 | 61 | 0.00000 |
| 1452 | 143 | TRP | CZ2 | -28.41151 | -28.41903 | 108.90296 | B1 | 61 | 0.00000 |
| 1453 | 143 | TRP | CZ3 | -28.94655 | -30.73482 | 108.27096 | B1 | 61 | 0.00000 |
| 1454 | 143 | TRP | CH2 | -29.03488 | -29.34388 | 108.03833 | B1 | 61 | 0.00000 |
| 1455 | 143 | TRP | C | -25.40824 | -32.93379 | 114.07770 | B1 | 61 | 0.00000 |
| 1456 | 143 | TRP | O | -26.13451 | -33.11650 | 115.04995 | B1 | 61 | 0.00000 |
| 1457 | 144 | ASN | N | -24.46546 | -33.80055 | 113.69236 | B1 | 62 | 0.00000 |
| 1458 | 144 | ASN | H | -23.94027 | -33.62305 | 112.85783 | B1 | 62 | 0.00000 |
| 1459 | 144 | ASN | CA | -24.16067 | -34.99080 | 114.49069 | B1 | 62 | 0.00000 |
| 1460 | 144 | ASN | CB | -23.20850 | -35.93308 | 113.73882 | B1 | 62 | 0.00000 |
| 1461 | 144 | ASN | CG | -23.89541 | -36.68861 | 112.61740 | B1 | 62 | 0.00000 |
| 1462 | 144 | ASN | OD1 | -23.68155 | -36.47075 | 111.43371 | B1 | 62 | 0.00000 |
| 1463 | 144 | ASN | ND2 | -24.72776 | -37.64097 | 113.02365 | B1 | 62 | 0.00000 |
| 1464 | 144 | ASN | HD21 | -24.89338 | -37.81926 | 113.99276 | B1 | 62 | 0.00000 |
| 1465 | 144 | ASN | HD22 | -25.19584 | -38.20406 | 112.34455 | B1 | 62 | 0.00000 |
| 1466 | 144 | ASN | C | -23.49875 | -34.69497 | 115.82591 | B1 | 62 | 0.00000 |
| 1467 | 144 | ASN | O | -23.43003 | -35.54654 | 116.69934 | B1 | 62 | 0.00000 |
| 1468 | 145 | SER | N | -22.99604 | -33.46640 | 115.97350 | B1 | 63 | 0.00000 |

FIG. 24

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1469 | 145 | SER | H | 22.97830 | -32.80428 | 115.21961 | B1 | 63 | 0.00000 |
| 1470 | 145 | SER | CA | 22.38004 | -33.14621 | 117.25865 | B1 | 63 | 0.00000 |
| 1471 | 145 | SER | CB | -20.91921 | -32.73054 | 117.01176 | B1 | 63 | 0.00000 |
| 1472 | 145 | SER | OG | -20.18983 | -32.64180 | 118.24511 | B1 | 63 | 0.00000 |
| 1473 | 145 | SER | HG | -20.76055 | -32.22535 | 118.91065 | B1 | 63 | 0.00000 |
| 1474 | 145 | SER | C | -23.11027 | -32.07614 | 118.06161 | B1 | 63 | 0.00000 |
| 1475 | 145 | SER | O | -22.67401 | -31.68287 | 119.13941 | B1 | 63 | 0.00000 |
| 1476 | 146 | GLN | N | -24.22180 | -31.59037 | 117.51252 | B1 | 64 | 0.00000 |
| 1477 | 146 | GLN | H | -24.58118 | -31.94604 | 116.64774 | B1 | 64 | 0.00000 |
| 1478 | 146 | GLN | CA | -24.90025 | -30.49286 | 118.19522 | B1 | 64 | 0.00000 |
| 1479 | 146 | GLN | CB | -24.86315 | -29.29301 | 117.23892 | B1 | 64 | 0.00000 |
| 1480 | 146 | GLN | CG | -25.45855 | -27.96945 | 117.72882 | B1 | 64 | 0.00000 |
| 1481 | 146 | GLN | CD | -26.89096 | -27.81462 | 117.25234 | B1 | 64 | 0.00000 |
| 1482 | 146 | GLN | OE1 | -27.80837 | -27.53609 | 118.00911 | B1 | 64 | 0.00000 |
| 1483 | 146 | GLN | NE2 | -27.06556 | -27.97948 | 115.94329 | B1 | 64 | 0.00000 |
| 1484 | 146 | GLN | HE21 | -26.30809 | -28.20349 | 115.33276 | B1 | 64 | 0.00000 |
| 1485 | 146 | GLN | HE22 | -27.98288 | -27.88997 | 115.56134 | B1 | 64 | 0.00000 |
| 1486 | 146 | GLN | C | -26.29488 | -30.93694 | 118.57642 | B1 | 64 | 0.00000 |
| 1487 | 146 | GLN | O | -27.21649 | -30.91839 | 117.77294 | B1 | 64 | 0.00000 |
| 1488 | 147 | LYS | N | -26.36947 | -31.44426 | 119.82371 | B1 | 65 | 0.00000 |
| 1489 | 147 | LYS | H | -25.65249 | -31.20699 | 120.47663 | B1 | 65 | 0.00000 |
| 1490 | 147 | LYS | CA | -27.35463 | -32.46614 | 120.21964 | B1 | 65 | 0.00000 |
| 1491 | 147 | LYS | CB | -28.27258 | -32.00851 | 121.37895 | B1 | 65 | 0.00000 |
| 1492 | 147 | LYS | CG | -29.34716 | -33.02726 | 121.84203 | B1 | 65 | 0.00000 |
| 1493 | 147 | LYS | CD | -28.88674 | -34.49172 | 121.97244 | B1 | 65 | 0.00000 |
| 1494 | 147 | LYS | CE | -29.96618 | -35.46785 | 121.47444 | B1 | 65 | 0.00000 |
| 1495 | 147 | LYS | NZ | -29.40221 | -36.81034 | 121.26907 | B1 | 65 | 0.00000 |
| 1496 | 147 | LYS | HZ1 | -30.04886 | -37.42223 | 120.71767 | B1 | 65 | 0.00000 |
| 1497 | 147 | LYS | HZ2 | -28.53282 | -36.76558 | 120.68922 | B1 | 65 | 0.00000 |
| 1498 | 147 | LYS | HZ3 | -29.15199 | -37.28892 | 122.15073 | B1 | 65 | 0.00000 |
| 1499 | 147 | LYS | C | -28.12445 | -33.12689 | 119.09340 | B1 | 65 | 0.00000 |
| 1500 | 147 | LYS | O | -29.30235 | -32.90174 | 118.83883 | B1 | 65 | 0.00000 |
| 1501 | 148 | ASP | N | -27.34620 | -34.00916 | 118.45822 | B1 | 66 | 0.00000 |
| 1502 | 148 | ASP | H | -26.39747 | -34.14495 | 118.75300 | B1 | 66 | 0.00000 |
| 1503 | 148 | ASP | CA | -27.79510 | -35.00236 | 117.48362 | B1 | 66 | 0.00000 |
| 1504 | 148 | ASP | CB | -27.88927 | -36.37833 | 118.17059 | B1 | 66 | 0.00000 |
| 1505 | 148 | ASP | CG | -26.79528 | -36.57930 | 119.21585 | B1 | 66 | 0.00000 |
| 1506 | 148 | ASP | OD1 | -25.69280 | -36.06325 | 119.05193 | B1 | 66 | 0.00000 |
| 1507 | 148 | ASP | OD2 | -27.07650 | -37.20742 | 120.23524 | B1 | 66 | 0.00000 |
| 1508 | 148 | ASP | C | -29.08887 | -34.63043 | 116.79645 | B1 | 66 | 0.00000 |
| 1509 | 148 | ASP | O | -30.17136 | -35.14808 | 117.04951 | B1 | 66 | 0.00000 |
| 1510 | 149 | LEU | N | -28.92399 | -33.61840 | 115.93941 | B1 | 67 | 0.00000 |
| 1511 | 149 | LEU | H | -27.98965 | -33.30949 | 115.73440 | B1 | 67 | 0.00000 |
| 1512 | 149 | LEU | CA | -30.07076 | -32.84836 | 115.45008 | B1 | 67 | 0.00000 |
| 1513 | 149 | LEU | CB | -29.45399 | -31.74267 | 114.57360 | B1 | 67 | 0.00000 |
| 1514 | 149 | LEU | CG | -30.29432 | -30.58223 | 114.02475 | B1 | 67 | 0.00000 |
| 1515 | 149 | LEU | CD1 | -30.85820 | -30.92475 | 112.65290 | B1 | 67 | 0.00000 |
| 1516 | 149 | LEU | CD2 | -31.34761 | -30.09615 | 115.02072 | B1 | 67 | 0.00000 |
| 1517 | 149 | LEU | C | -31.17667 | -33.69413 | 114.80952 | B1 | 67 | 0.00000 |
| 1518 | 149 | LEU | O | -32.36472 | -33.37859 | 114.83807 | B1 | 67 | 0.00000 |
| 1519 | 150 | LEU | N | -30.73118 | -34.86138 | 114.32363 | B1 | 68 | 0.00000 |
| 1520 | 150 | LEU | H | -29.75579 | -34.94139 | 114.11621 | B1 | 68 | 0.00000 |
| 1521 | 150 | LEU | CA | -31.59782 | -36.02822 | 114.12850 | B1 | 68 | 0.00000 |
| 1522 | 150 | LEU | CB | -30.74740 | -37.29867 | 114.15286 | B1 | 68 | 0.00000 |
| 1523 | 150 | LEU | CG | -29.89363 | -37.44772 | 112.89569 | B1 | 68 | 0.00000 |
| 1524 | 150 | LEU | CD1 | -29.64060 | -38.26626 | 113.18796 | B1 | 68 | 0.00000 |
| 1525 | 150 | LEU | CD2 | -30.71709 | -38.01712 | 111.73915 | B1 | 68 | 0.00000 |
| 1526 | 150 | LEU | C | -32.74973 | -36.17247 | 115.10785 | B1 | 68 | 0.00000 |
| 1527 | 150 | LEU | O | -33.89001 | -36.01901 | 114.70350 | B1 | 68 | 0.00000 |
| 1528 | 151 | GLU | N | -32.47441 | -36.43576 | 116.39428 | B1 | 69 | 0.00000 |
| 1529 | 151 | GLU | H | -31.52943 | -36.57284 | 116.72119 | B1 | 69 | 0.00000 |
| 1530 | 151 | GLU | CA | -33.61295 | -36.59512 | 117.30950 | B1 | 69 | 0.00000 |
| 1531 | 151 | GLU | CB | -33.19489 | -36.98331 | 118.72928 | B1 | 69 | 0.00000 |
| 1532 | 151 | GLU | CG | -32.69081 | -38.41906 | 118.86324 | B1 | 69 | 0.00000 |

FIG. 25

./[illegible]_GLN2.CRD Thu Feb 25 14:58:48 1993 25

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1533 | 151 | GLU | CD | -31.19287 | -38.44464 | 118.70497 | B1 | 69 | 0.00000 |
| 1534 | 151 | GLU | OE1 | -30.71320 | -38.33129 | 117.58148 | B1 | 69 | 0.00000 |
| 1535 | 151 | GLU | OE2 | -30.51522 | -38.56462 | 119.72459 | B1 | 69 | 0.00000 |
| 1536 | 151 | GLU | C | -34.55067 | -35.41168 | 117.43857 | B1 | 69 | 0.00000 |
| 1537 | 151 | GLU | O | -35.75790 | -35.57313 | 117.58647 | B1 | 69 | 0.00000 |
| 1538 | 152 | GLN | N | -33.98601 | -34.19700 | 117.35586 | B1 | 70 | 0.00000 |
| 1539 | 152 | GLN | H | -33.00321 | -34.10256 | 117.18602 | B1 | 70 | 0.00000 |
| 1540 | 152 | GLN | CA | -34.89656 | -33.04752 | 117.40695 | B1 | 70 | 0.00000 |
| 1541 | 152 | GLN | CB | -34.15680 | -31.71646 | 117.32018 | B1 | 70 | 0.00000 |
| 1542 | 152 | GLN | CG | -33.46159 | -31.26900 | 118.60094 | B1 | 70 | 0.00000 |
| 1543 | 152 | GLN | CD | -33.23376 | -29.77424 | 118.49387 | B1 | 70 | 0.00000 |
| 1544 | 152 | GLN | OE1 | -32.13068 | -29.27019 | 118.36008 | B1 | 70 | 0.00000 |
| 1545 | 152 | GLN | NE2 | -34.34656 | -29.04662 | 118.54711 | B1 | 70 | 0.00000 |
| 1546 | 152 | GLN | HE21 | -35.24607 | -29.46511 | 118.65663 | B1 | 70 | 0.00000 |
| 1547 | 152 | GLN | HE22 | -34.28188 | -28.05358 | 118.46911 | B1 | 70 | 0.00000 |
| 1548 | 152 | GLN | C | -35.89575 | -33.04746 | 116.27182 | B1 | 70 | 0.00000 |
| 1549 | 152 | GLN | O | -37.09756 | -32.85841 | 116.43607 | B1 | 70 | 0.00000 |
| 1550 | 153 | ARG | N | -35.34435 | -33.30759 | 115.08552 | B1 | 71 | 0.00000 |
| 1551 | 153 | ARG | H | -34.35839 | -33.48709 | 114.99299 | B1 | 71 | 0.00000 |
| 1552 | 153 | ARG | CA | -36.25853 | -33.42129 | 113.95947 | B1 | 71 | 0.00000 |
| 1553 | 153 | ARG | CB | -35.46322 | -33.43707 | 112.66564 | B1 | 71 | 0.00000 |
| 1554 | 153 | ARG | CG | -34.84280 | -32.07791 | 112.35054 | B1 | 71 | 0.00000 |
| 1555 | 153 | ARG | CD | -33.88499 | -32.22570 | 111.17839 | B1 | 71 | 0.00000 |
| 1556 | 153 | ARG | NE | -33.53171 | -30.95306 | 110.55166 | B1 | 71 | 0.00000 |
| 1557 | 153 | ARG | HE | -33.78858 | -30.09360 | 110.98860 | B1 | 71 | 0.00000 |
| 1558 | 153 | ARG | CZ | -33.01475 | -31.01372 | 109.31716 | B1 | 71 | 0.00000 |
| 1559 | 153 | ARG | NH1 | -32.97943 | -29.92906 | 108.54980 | B1 | 71 | 0.00000 |
| 1560 | 153 | ARG | HH11 | -32.81618 | -30.04802 | 107.55422 | B1 | 71 | 0.00000 |
| 1561 | 153 | ARG | HH12 | -33.14801 | -29.01024 | 108.90136 | B1 | 71 | 0.00000 |
| 1562 | 153 | ARG | NH2 | -32.57787 | -32.17691 | 108.83735 | B1 | 71 | 0.00000 |
| 1563 | 153 | ARG | HH21 | -32.40269 | -32.29042 | 107.04355 | B1 | 71 | 0.00000 |
| 1564 | 153 | ARG | HH22 | -32.45571 | -32.97359 | 109.42307 | B1 | 71 | 0.00000 |
| 1565 | 153 | ARG | C | -37.16363 | -34.62908 | 114.06926 | B1 | 71 | 0.00000 |
| 1566 | 153 | ARG | O | -38.37029 | -34.50228 | 113.96948 | B1 | 71 | 0.00000 |
| 1567 | 154 | ARG | N | -36.57082 | -35.79410 | 114.34589 | B1 | 72 | 0.00000 |
| 1568 | 154 | ARG | H | -35.57655 | -35.83805 | 114.34685 | B1 | 72 | 0.00000 |
| 1569 | 154 | ARG | CA | -37.32441 | -37.02834 | 114.59374 | B1 | 72 | 0.00000 |
| 1570 | 154 | ARG | CB | -36.30581 | -38.11823 | 115.12926 | B1 | 72 | 0.00000 |
| 1571 | 154 | ARG | CG | -37.06240 | -39.48786 | 115.22908 | B1 | 72 | 0.00000 |
| 1572 | 154 | ARG | CD | -36.14056 | -40.61269 | 115.69023 | B1 | 72 | 0.00000 |
| 1573 | 154 | ARG | NE | -36.90866 | -41.85162 | 115.80184 | B1 | 72 | 0.00000 |
| 1574 | 154 | ARG | HE | -37.59626 | -42.01330 | 115.09038 | B1 | 72 | 0.00000 |
| 1575 | 154 | ARG | CZ | -36.70093 | -42.71372 | 116.80504 | B1 | 72 | 0.00000 |
| 1576 | 154 | ARG | NH1 | -37.45795 | -43.80593 | 116.88687 | B1 | 72 | 0.00000 |
| 1577 | 154 | ARG | HH11 | -37.33416 | -44.47837 | 117.61587 | B1 | 72 | 0.00000 |
| 1578 | 154 | ARG | HH12 | -38.17495 | -43.96809 | 116.20728 | B1 | 72 | 0.00000 |
| 1579 | 154 | ARG | NH2 | -35.75363 | -42.48325 | 117.71513 | B1 | 72 | 0.00000 |
| 1580 | 154 | ARG | HH21 | -35.59042 | -43.10493 | 118.48012 | B1 | 72 | 0.00000 |
| 1581 | 154 | ARG | HH22 | -35.18100 | -41.66590 | 117.63709 | B1 | 72 | 0.00000 |
| 1582 | 154 | ARG | C | -38.52465 | -36.88141 | 115.51516 | B1 | 72 | 0.00000 |
| 1583 | 154 | ARG | O | -39.58964 | -37.43301 | 115.28503 | B1 | 72 | 0.00000 |
| 1584 | 155 | ARG | N | -38.35223 | -36.06670 | 116.55472 | B1 | 73 | 0.00000 |
| 1585 | 155 | ARG | H | -37.44332 | -35.69920 | 116.77047 | B1 | 73 | 0.00000 |
| 1586 | 155 | ARG | CA | -39.52250 | -35.72569 | 117.36371 | B1 | 73 | 0.00000 |
| 1587 | 155 | ARG | CB | -39.05476 | -34.79593 | 118.48265 | B1 | 73 | 0.00000 |
| 1588 | 155 | ARG | CG | -40.15723 | -34.36970 | 119.44775 | B1 | 73 | 0.00000 |
| 1589 | 155 | ARG | CD | -39.62900 | -33.36327 | 120.46128 | B1 | 73 | 0.00000 |
| 1590 | 155 | ARG | NE | -40.71623 | -32.83780 | 121.28237 | B1 | 73 | 0.00000 |
| 1591 | 155 | ARG | HE | -41.63763 | -33.18145 | 121.09517 | B1 | 73 | 0.00000 |
| 1592 | 155 | ARG | CZ | -40.47089 | -31.92135 | 122.22743 | B1 | 73 | 0.00000 |
| 1593 | 155 | ARG | NH1 | -41.48382 | -31.43599 | 122.94081 | B1 | 73 | 0.00000 |
| 1594 | 155 | ARG | HH11 | -41.33888 | -30.75247 | 123.65592 | B1 | 73 | 0.00000 |
| 1595 | 155 | ARG | HH12 | -42.41818 | -31.75018 | 122.77039 | B1 | 73 | 0.00000 |
| 1596 | 155 | ARG | NH2 | -39.22715 | -31.49669 | 122.45304 | B1 | 73 | 0.00000 |

FIG. 26

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1661 | 162 | ARG | NE | 50.49694 | -40.88455 | 114.11092 | B1 | 80 | 0.00000 |
| 1662 | 162 | ARG | CZ | 49.34267 | -42.40507 | 114.80601 | B1 | 80 | 0.00000 |
| 1663 | 162 | ARG | NH1 | -50.23020 | -43.32564 | 114.46730 | B1 | 80 | 0.00000 |
| 1664 | 162 | ARG | HH11 | -50.11979 | -44.31403 | 114.66150 | B1 | 80 | 0.00000 |
| 1665 | 162 | ARG | HH12 | -51.06184 | -43.06285 | 113.96028 | B1 | 80 | 0.00000 |
| 1666 | 162 | ARG | NH2 | -48.19839 | -42.76163 | 115.38323 | B1 | 80 | 0.00000 |
| 1667 | 162 | ARG | HH21 | -48.00134 | -43.72771 | 115.55650 | B1 | 80 | 0.00000 |
| 1668 | 162 | ARG | HH22 | -47.52579 | -42.06788 | 115.64161 | B1 | 80 | 0.00000 |
| 1669 | 162 | ARG | C | -49.75512 | -35.92906 | 113.42487 | B1 | 80 | 0.00000 |
| 1670 | 162 | ARG | O | -50.82093 | -35.93732 | 112.81658 | B1 | 80 | 0.00000 |
| 1671 | 163 | HIS | N | -49.58593 | -35.31862 | 114.60088 | B1 | 81 | 0.00000 |
| 1672 | 163 | HIS | H | -48.68252 | -35.28035 | 115.03933 | B1 | 81 | 0.00000 |
| 1673 | 163 | HIS | CA | -50.76431 | -34.73357 | 115.23467 | B1 | 81 | 0.00000 |
| 1674 | 163 | HIS | CB | -50.42874 | -34.29045 | 116.66134 | B1 | 81 | 0.00000 |
| 1675 | 163 | HIS | CG | -50.41026 | -35.50649 | 117.55950 | B1 | 81 | 0.00000 |
| 1676 | 163 | HIS | ND1 | -51.51644 | -36.01842 | 118.12240 | B1 | 81 | 0.00000 |
| 1677 | 163 | HIS | HD1 | -52.42830 | -35.67431 | 118.03242 | B1 | 81 | 0.00000 |
| 1678 | 163 | HIS | CD2 | -49.31404 | -36.28837 | 117.93420 | B1 | 81 | 0.00000 |
| 1679 | 163 | HIS | NE2 | -49.78030 | -37.28089 | 118.73130 | B1 | 81 | 0.00000 |
| 1680 | 163 | HIS | CE1 | -51.13423 | -37.11585 | 118.84798 | B1 | 81 | 0.00000 |
| 1681 | 163 | HIS | C | -51.37160 | -33.59588 | 114.44466 | B1 | 81 | 0.00000 |
| 1682 | 163 | HIS | O | -52.56947 | -33.55956 | 114.18659 | B1 | 81 | 0.00000 |
| 1683 | 164 | ASN | N | -50.50246 | -32.67616 | 114.01202 | B1 | 82 | 0.00000 |
| 1684 | 164 | ASN | H | -49.51981 | -32.74462 | 114.21247 | B1 | 82 | 0.00000 |
| 1685 | 164 | ASN | CA | -51.04300 | -31.58239 | 113.20331 | B1 | 82 | 0.00000 |
| 1686 | 164 | ASN | CB | -49.96583 | -30.54361 | 112.89196 | B1 | 82 | 0.00000 |
| 1687 | 164 | ASN | CG | -49.91907 | -29.53869 | 114.02377 | B1 | 82 | 0.00000 |
| 1688 | 164 | ASN | OD1 | -49.13948 | -29.62233 | 114.96163 | B1 | 82 | 0.00000 |
| 1689 | 164 | ASN | ND2 | -50.80473 | -28.55321 | 113.91309 | B1 | 82 | 0.00000 |
| 1690 | 164 | ASN | HD21 | -51.44311 | -28.49843 | 113.14586 | B1 | 82 | 0.00000 |
| 1691 | 164 | ASN | HD22 | -50.84210 | -27.84178 | 114.61251 | B1 | 82 | 0.00000 |
| 1692 | 164 | ASN | C | -51.70674 | -32.02333 | 111.91584 | B1 | 82 | 0.00000 |
| 1693 | 164 | ASN | O | -52.73418 | -31.48682 | 111.51085 | B1 | 82 | 0.00000 |
| 1694 | 165 | TYR | N | -51.12326 | -33.05626 | 111.29191 | B1 | 83 | 0.00000 |
| 1695 | 165 | TYR | H | -50.28201 | -33.49370 | 111.62194 | B1 | 83 | 0.00000 |
| 1696 | 165 | TYR | CA | -51.81304 | -33.54191 | 110.10401 | B1 | 83 | 0.00000 |
| 1697 | 165 | TYR | CB | -50.92781 | -34.47239 | 109.25048 | B1 | 83 | 0.00000 |
| 1698 | 165 | TYR | CG | -51.39689 | -34.50284 | 107.80317 | B1 | 83 | 0.00000 |
| 1699 | 165 | TYR | CD1 | -52.18946 | -33.44669 | 107.29137 | B1 | 83 | 0.00000 |
| 1700 | 165 | TYR | CE1 | -52.63312 | -33.47413 | 105.96126 | B1 | 83 | 0.00000 |
| 1701 | 165 | TYR | CD2 | -51.04289 | -35.58963 | 106.96903 | B1 | 83 | 0.00000 |
| 1702 | 165 | TYR | CE2 | -51.48846 | -35.61522 | 105.62740 | B1 | 83 | 0.00000 |
| 1703 | 165 | TYR | CZ | -52.28557 | -34.55457 | 105.13440 | B1 | 83 | 0.00000 |
| 1704 | 165 | TYR | OH | -52.75931 | -34.53152 | 103.84155 | B1 | 83 | 0.00000 |
| 1705 | 165 | TYR | HH | -52.13515 | -34.97162 | 103.24416 | B1 | 83 | 0.00000 |
| 1706 | 165 | TYR | C | -53.16114 | -34.17050 | 110.39688 | B1 | 83 | 0.00000 |
| 1707 | 165 | TYR | O | -54.17243 | -33.75040 | 109.85354 | B1 | 83 | 0.00000 |
| 1708 | 166 | GLY | N | -53.16827 | -35.13255 | 111.32677 | B1 | 84 | 0.00000 |
| 1709 | 166 | GLY | H | -52.30920 | -35.44284 | 111.74443 | B1 | 84 | 0.00000 |
| 1710 | 166 | GLY | CA | -54.44388 | -35.75931 | 111.69489 | B1 | 84 | 0.00000 |
| 1711 | 166 | GLY | C | -55.55421 | -34.78683 | 112.08191 | B1 | 84 | 0.00000 |
| 1712 | 166 | GLY | O | -56.70058 | -34.86763 | 111.64884 | B1 | 84 | 0.00000 |
| 1713 | 167 | VAL | N | -55.16433 | -33.81049 | 112.90998 | B1 | 85 | 0.00000 |
| 1714 | 167 | VAL | H | -54.21931 | -33.77699 | 113.25020 | B1 | 85 | 0.00000 |
| 1715 | 167 | VAL | CA | -56.14083 | -32.77588 | 113.26808 | B1 | 85 | 0.00000 |
| 1716 | 167 | VAL | CB | -55.54422 | -31.87200 | 114.36486 | B1 | 85 | 0.00000 |
| 1717 | 167 | VAL | CG1 | -56.46931 | -30.71890 | 114.75691 | B1 | 85 | 0.00000 |
| 1718 | 167 | VAL | CG2 | -55.22649 | -32.70528 | 115.60849 | B1 | 85 | 0.00000 |
| 1719 | 167 | VAL | C | -56.62003 | -31.96437 | 112.06515 | B1 | 85 | 0.00000 |
| 1720 | 167 | VAL | O | -57.80658 | -31.70971 | 111.87365 | B1 | 85 | 0.00000 |
| 1721 | 168 | GLY | N | -55.65605 | -31.61592 | 111.20320 | B1 | 86 | 0.00000 |
| 1722 | 168 | GLY | H | -54.68827 | -31.81924 | 111.38362 | B1 | 86 | 0.00000 |
| 1723 | 168 | GLY | CA | -56.04215 | -30.96490 | 109.94972 | B1 | 86 | 0.00000 |
| 1724 | 168 | GLY | C | -57.02338 | -31.77629 | 109.11607 | B1 | 86 | 0.00000 |

FIG. 28

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1725 | 168 | GLY | O | 58.02649 | -31.28044 | 108.61617 | B1 | 86 | 0.00000 |
| 1726 | 169 | GLU | N | 56.71134 | -33.07169 | 109.00665 | B1 | 87 | 0.00000 |
| 1727 | 169 | GLU | H | -55.87921 | -33.43085 | 109.43169 | B1 | 87 | 0.00000 |
| 1728 | 169 | GLU | CA | -57.59179 | -34.00467 | 108.30469 | B1 | 87 | 0.00000 |
| 1729 | 169 | GLU | CB | -56.95070 | -35.39155 | 108.28846 | B1 | 87 | 0.00000 |
| 1730 | 169 | GLU | CG | -55.67851 | -35.40281 | 107.43481 | B1 | 87 | 0.00000 |
| 1731 | 169 | GLU | CD | -54.91259 | -36.69049 | 107.65905 | B1 | 87 | 0.00000 |
| 1732 | 169 | GLU | OE1 | -53.74095 | -36.61342 | 108.02205 | B1 | 87 | 0.00000 |
| 1733 | 169 | GLU | OE2 | -55.48540 | -37.76250 | 107.47736 | B1 | 87 | 0.00000 |
| 1734 | 169 | GLU | C | -59.00151 | -34.05273 | 108.86565 | B1 | 87 | 0.00000 |
| 1735 | 169 | GLU | O | -59.98966 | -34.06690 | 108.14126 | B1 | 87 | 0.00000 |
| 1736 | 170 | SER | N | -59.06996 | -33.99305 | 110.19884 | B1 | 88 | 0.00000 |
| 1737 | 170 | SER | H | -58.23138 | -34.05998 | 110.74831 | B1 | 88 | 0.00000 |
| 1738 | 170 | SER | CA | -60.38255 | -33.85094 | 110.83391 | B1 | 88 | 0.00000 |
| 1739 | 170 | SER | CB | -60.18950 | -33.85581 | 112.35798 | B1 | 88 | 0.00000 |
| 1740 | 170 | SER | OG | -61.42043 | -34.13237 | 113.03659 | B1 | 88 | 0.00000 |
| 1741 | 170 | SER | HG | -61.30877 | -34.00943 | 113.98374 | B1 | 88 | 0.00000 |
| 1742 | 170 | SER | C | -61.16415 | -32.61665 | 110.37646 | B1 | 88 | 0.00000 |
| 1743 | 170 | SER | O | -62.31497 | -32.69150 | 109.96191 | B1 | 88 | 0.00000 |
| 1744 | 171 | PHE | N | -60.49231 | -31.45621 | 110.41676 | B1 | 89 | 0.00000 |
| 1745 | 171 | PHE | H | -59.54601 | -31.41832 | 110.75393 | B1 | 89 | 0.00000 |
| 1746 | 171 | PHE | CA | -61.19539 | -30.24631 | 109.95663 | B1 | 89 | 0.00000 |
| 1747 | 171 | PHE | CB | -60.30793 | -28.99941 | 110.10880 | B1 | 89 | 0.00000 |
| 1748 | 171 | PHE | CG | -59.94208 | -28.68147 | 111.54294 | B1 | 89 | 0.00000 |
| 1749 | 171 | PHE | CD1 | -58.59291 | -28.39703 | 111.85413 | B1 | 89 | 0.00000 |
| 1750 | 171 | PHE | CD2 | -60.93098 | -28.63398 | 112.55491 | B1 | 89 | 0.00000 |
| 1751 | 171 | PHE | CE1 | -58.23032 | -28.06074 | 113.17656 | B1 | 89 | 0.00000 |
| 1752 | 171 | PHE | CE2 | -60.56845 | -28.29967 | 113.87858 | B1 | 89 | 0.00000 |
| 1753 | 171 | PHE | CZ | -59.21901 | -28.01319 | 114.18527 | B1 | 89 | 0.00000 |
| 1754 | 171 | PHE | C | -61.62802 | -30.29139 | 108.49502 | B1 | 89 | 0.00000 |
| 1755 | 171 | PHE | O | -62.68697 | -29.84047 | 108.07691 | B1 | 89 | 0.00000 |
| 1756 | 172 | THR | N | -60.72520 | -30.85206 | 107.69903 | B1 | 90 | 0.00000 |
| 1757 | 172 | THR | H | -59.91792 | -31.29854 | 108.09636 | B1 | 90 | 0.00000 |
| 1758 | 172 | THR | CA | -60.04308 | -30.66246 | 106.25599 | B1 | 90 | 0.00000 |
| 1759 | 172 | THR | CB | -59.41710 | -30.70747 | 105.70165 | B1 | 90 | 0.00000 |
| 1760 | 172 | THR | OG1 | -59.35292 | -30.21143 | 104.36207 | B1 | 90 | 0.00000 |
| 1761 | 172 | THR | HG1 | -60.15430 | -30.48800 | 103.89285 | B1 | 90 | 0.00000 |
| 1762 | 172 | THR | CG2 | -58.90262 | -32.13906 | 105.74825 | B1 | 90 | 0.00000 |
| 1763 | 172 | THR | C | -61.71208 | -31.64877 | 105.47987 | B1 | 90 | 0.00000 |
| 1764 | 172 | THR | O | -61.76078 | -31.56505 | 104.25169 | B1 | 90 | 0.00000 |
| 1765 | 173 | VAL | N | -62.32957 | -32.60764 | 106.19315 | B1 | 91 | 0.00000 |
| 1766 | 173 | VAL | H | -62.28706 | -32.56397 | 107.19363 | B1 | 91 | 0.00000 |
| 1767 | 173 | VAL | CA | -62.87984 | -33.81113 | 105.53718 | B1 | 91 | 0.00000 |
| 1768 | 173 | VAL | CB | -63.87967 | -34.51911 | 106.47899 | B1 | 91 | 0.00000 |
| 1769 | 173 | VAL | CG1 | -64.50006 | -35.77324 | 105.85034 | B1 | 91 | 0.00000 |
| 1770 | 173 | VAL | CG2 | -63.20452 | -34.90248 | 107.79466 | B1 | 91 | 0.00000 |
| 1771 | 173 | VAL | C | -63.51710 | -33.59419 | 104.16716 | B1 | 91 | 0.00000 |
| 1772 | 173 | VAL | O | -63.18750 | -34.24452 | 103.18126 | B1 | 91 | 0.00000 |
| 1773 | 174 | GLN | N | -64.41211 | -32.59570 | 104.14711 | B1 | 92 | 0.00000 |
| 1774 | 174 | GLN | H | -64.59818 | -32.11269 | 105.00138 | B1 | 92 | 0.00000 |
| 1775 | 174 | GLN | CA | -65.14373 | -32.19104 | 102.94243 | B1 | 92 | 0.00000 |
| 1776 | 174 | GLN | CB | -65.76132 | -30.80951 | 103.22574 | B1 | 92 | 0.00000 |
| 1777 | 174 | GLN | CG | -66.77986 | -30.26016 | 102.21318 | B1 | 92 | 0.00000 |
| 1778 | 174 | GLN | CD | -66.09397 | -29.58024 | 101.04012 | B1 | 92 | 0.00000 |
| 1779 | 174 | GLN | OE1 | -65.45924 | -28.54065 | 101.15380 | B1 | 92 | 0.00000 |
| 1780 | 174 | GLN | NE2 | -66.26402 | -30.18961 | 99.87453 | B1 | 92 | 0.00000 |
| 1781 | 174 | GLN | HE21 | -66.63226 | -31.11966 | 99.82928 | B1 | 92 | 0.00000 |
| 1782 | 174 | GLN | HE22 | -65.97833 | -29.74839 | 99.02730 | B1 | 92 | 0.00000 |
| 1783 | 174 | GLN | C | -64.36067 | -32.18074 | 101.63553 | B1 | 92 | 0.00000 |
| 1784 | 174 | GLN | O | -64.88582 | -32.51356 | 100.57991 | B1 | 92 | 0.00000 |
| 1785 | 175 | ARG | N | -63.09233 | -31.77447 | 101.73327 | B1 | 93 | 0.00000 |
| 1786 | 175 | ARG | H | -62.69754 | -31.53564 | 102.62225 | B1 | 93 | 0.00000 |
| 1787 | 175 | ARG | CA | -62.31707 | -31.78835 | 100.50018 | B1 | 93 | 0.00000 |
| 1788 | 175 | ARG | CB | -61.85817 | -30.36631 | 100.16958 | B1 | 93 | 0.00000 |

FIG. 29

../DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 29

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1789 | 175 | ARG | CG | -61.24395 | -30.26914 | 90.77310 | B1 | 93 | 0.00000 |
| 1790 | 175 | ARG | CD | -60.91597 | -28.04209 | 98.34709 | B1 | 93 | 0.00000 |
| 1791 | 175 | ARG | NE | -59.98117 | -28.87216 | 97.22615 | B1 | 93 | 0.00000 |
| 1792 | 175 | ARG | HE | -59.59146 | -29.76910 | 97.00518 | B1 | 93 | 0.00000 |
| 1793 | 175 | ARG | CZ | -59.49795 | -27.74924 | 96.68186 | B1 | 93 | 0.00000 |
| 1794 | 175 | ARG | NH1 | -58.57343 | -27.83579 | 95.72833 | B1 | 93 | 0.00000 |
| 1795 | 175 | ARG | HH11 | -58.19414 | -27.02728 | 95.28229 | B1 | 93 | 0.00000 |
| 1796 | 175 | ARG | HH12 | -58.22480 | -28.73459 | 95.46034 | B1 | 93 | 0.00000 |
| 1797 | 175 | ARG | NH2 | -59.92427 | -26.55682 | 97.09593 | B1 | 93 | 0.00000 |
| 1798 | 175 | ARG | HH21 | -59.57028 | -25.70796 | 96.70808 | B1 | 93 | 0.00000 |
| 1799 | 175 | ARG | HH22 | -60.60311 | -26.50975 | 97.82696 | B1 | 93 | 0.00000 |
| 1800 | 175 | ARG | C | -61.17336 | -32.79150 | 100.46150 | B1 | 93 | 0.00000 |
| 1801 | 175 | ARG | O | -61.02327 | -33.52738 | 99.49809 | B1 | 93 | 0.00000 |
| 1802 | 176 | ARG | N | -60.36493 | -32.85103 | 101.53216 | B1 | 94 | 0.00000 |
| 1803 | 176 | ARG | H | -60.53761 | -32.31340 | 102.35642 | B1 | 94 | 0.00000 |
| 1804 | 176 | ARG | CA | -59.25084 | -33.80802 | 101.41499 | B1 | 94 | 0.00000 |
| 1805 | 176 | ARG | CB | -58.18750 | -33.62483 | 102.49829 | B1 | 94 | 0.00000 |
| 1806 | 176 | ARG | CG | -57.32871 | -32.37173 | 102.34974 | B1 | 94 | 0.00000 |
| 1807 | 176 | ARG | CD | -56.27515 | -32.28237 | 103.45854 | B1 | 94 | 0.00000 |
| 1808 | 176 | ARG | NE | -56.30062 | -30.94018 | 104.04511 | B1 | 94 | 0.00000 |
| 1809 | 176 | ARG | HE | -56.83150 | -30.25818 | 103.53710 | B1 | 94 | 0.00000 |
| 1810 | 176 | ARG | CZ | -55.69078 | -30.63659 | 105.19759 | B1 | 94 | 0.00000 |
| 1811 | 176 | ARG | NH1 | -55.74431 | -29.38340 | 105.64628 | B1 | 94 | 0.00000 |
| 1812 | 176 | ARG | HH11 | -55.30471 | -29.10955 | 106.50132 | B1 | 94 | 0.00000 |
| 1813 | 176 | ARG | HH12 | -56.24080 | -28.69008 | 105.12278 | B1 | 94 | 0.00000 |
| 1814 | 176 | ARG | NH2 | -55.05038 | -31.57276 | 105.89297 | B1 | 94 | 0.00000 |
| 1815 | 176 | ARG | HH21 | -54.58912 | -31.37726 | 106.75753 | B1 | 94 | 0.00000 |
| 1816 | 176 | ARG | HH22 | -55.02183 | -32.51329 | 105.54660 | B1 | 94 | 0.00000 |
| 1817 | 176 | ARG | C | -59.64686 | -35.27348 | 101.42902 | B1 | 94 | 0.00000 |
| 1818 | 176 | ARG | O | -58.87808 | -36.15316 | 101.06767 | B1 | 94 | 0.00000 |
| 1819 | 177 | VAL | N | -60.88626 | -35.53390 | 101.85272 | B1 | 95 | 0.00000 |
| 1820 | 177 | VAL | H | -61.51901 | -34.82991 | 102.18430 | B1 | 95 | 0.00000 |
| 1821 | 177 | VAL | CA | -61.32863 | -36.91608 | 101.70299 | B1 | 95 | 0.00000 |
| 1822 | 177 | VAL | CB | -61.79519 | -37.47193 | 103.06780 | B1 | 95 | 0.00000 |
| 1823 | 177 | VAL | CG1 | -61.84113 | -39.00335 | 103.05589 | B1 | 95 | 0.00000 |
| 1824 | 177 | VAL | CG2 | -60.88761 | -37.00753 | 104.21299 | B1 | 95 | 0.00000 |
| 1825 | 177 | VAL | C | -62.41412 | -37.02458 | 100.63553 | B1 | 95 | 0.00000 |
| 1826 | 177 | VAL | O | -63.44404 | -37.67295 | 100.79118 | B1 | 95 | 0.00000 |
| 1827 | 178 | HIS | N | -62.14889 | -36.33028 | 99.52296 | B1 | 96 | 0.00000 |
| 1828 | 178 | HIS | H | -61.32158 | -35.77698 | 99.39184 | B1 | 96 | 0.00000 |
| 1829 | 178 | HIS | CA | -63.09845 | -36.32813 | 98.41659 | B1 | 96 | 0.00000 |
| 1830 | 178 | HIS | CB | -64.01495 | -35.10064 | 98.57314 | B1 | 96 | 0.00000 |
| 1831 | 178 | HIS | CG | -65.27852 | -35.21481 | 97.74669 | B1 | 96 | 0.00000 |
| 1832 | 178 | HIS | ND1 | -65.30573 | -35.62002 | 96.46944 | B1 | 96 | 0.00000 |
| 1833 | 178 | HIS | HD1 | -64.50806 | -35.91855 | 95.96816 | B1 | 96 | 0.00000 |
| 1834 | 178 | HIS | CD2 | -66.58524 | -34.92566 | 98.14872 | B1 | 96 | 0.00000 |
| 1835 | 178 | HIS | NE2 | -67.39749 | -35.16505 | 97.08780 | B1 | 96 | 0.00000 |
| 1836 | 178 | HIS | CE1 | -66.60728 | -35.59364 | 96.05191 | B1 | 96 | 0.00000 |
| 1837 | 178 | HIS | C | -62.34621 | -36.29235 | 97.09131 | B1 | 96 | 0.00000 |
| 1838 | 178 | HIS | OCT1 | -61.22615 | -35.78756 | 97.07091 | B1 | 96 | 0.00000 |
| 1839 | 178 | HIS | OCT2 | -62.87363 | -36.77415 | 96.08799 | B1 | 96 | 0.00000 |

FIG. 30

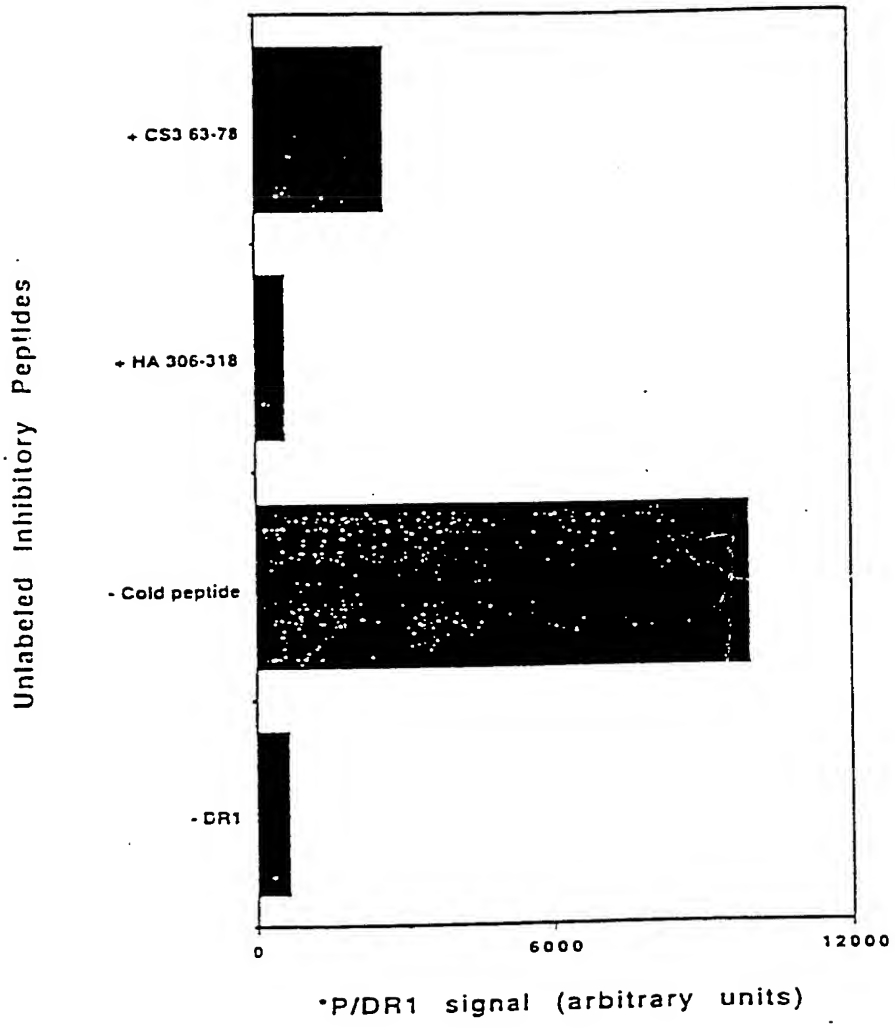
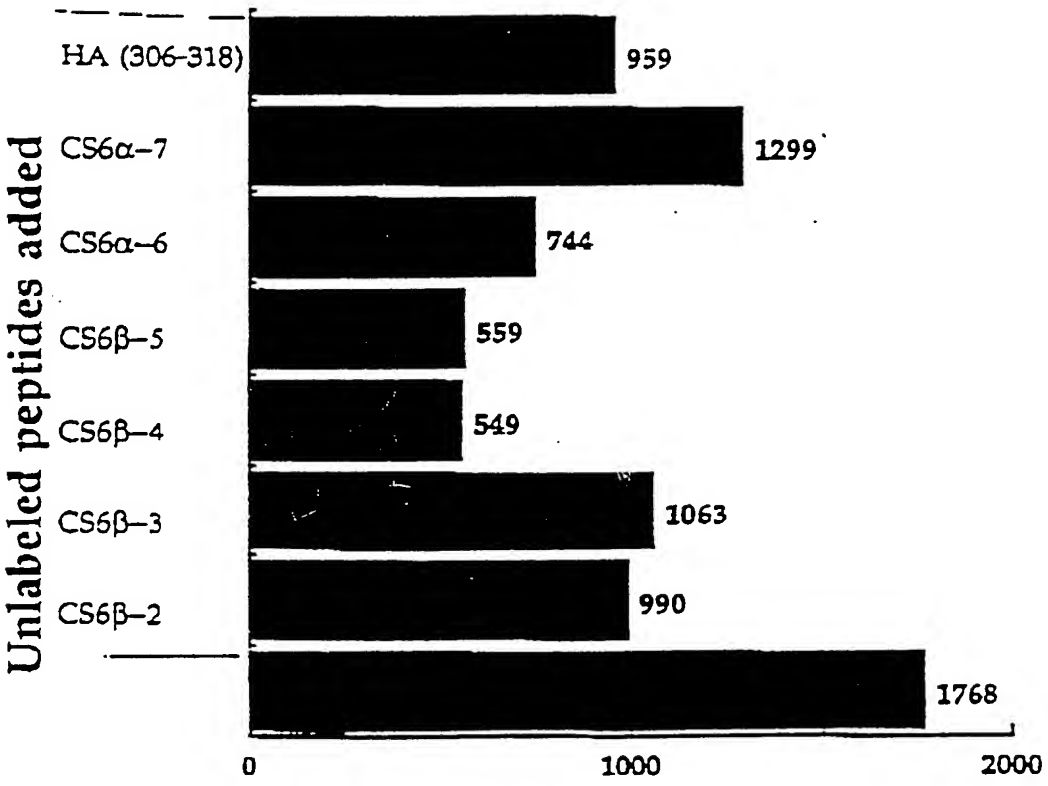

Unlabeled Inhibitory Peptides
+ CS3 63-78
+ HA 306-318
- Cold peptide
- DR1
0
6000
12000
*P/DR1 signal (arbitrary units)

FIG. 31

Inhibition of $^{125}$I HA(306-318)/DR1 by unlabeled CS6 α and β peptides




*HA/DR1 compact dimer signal (densitometric units)

FIG. 32

# INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

**A. CLASSIFICATION OF SUBJECT MATTER**

IPC(5) :A61K 39/00, 39/02, 39/12, 37/02, 35/14
US CL :424/185.1, 186.1, 190.1, 242.1; 530/327, 326, 333, 334, 388.75
According to International Patent Classification (IPC) or to both national classification and IPC

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 424/185.1, 186.1, 190.1, 242.1; 530/327, 326, 333, 334, 388.75

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| X | The Journal of Immunology, Volume 150, No. 8, Part II, issued 15 April 1993, Nauss et al., " Binding Interactions of Peptides in a Structural Homology Model of the DR1 Class MHC ", page 41A, Abstract 221, see entire abstract. | 1, 3-20 |
| X<br>----<br>Y | Nature, Volume 358, issued 27 August 1992, Chicz et al., "Predominant Naturally Processed Peptides Bound to HLA-DR1 are derived from MHC-related Molecule and are Heterogenous in Size", pages 764-768, see page 766, Table 2, and Table 3. | 12<br>------<br>1, 3-7 |

[X] Further documents are listed in the continuation of Box C. [ ] See patent family annex.

| | | | |
|---|---|---|---|
| * | Special categories of cited documents: | "T" | later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention |
| "A" | document defining the general state of the art which is not considered to be of particular relevance | "X" | document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone |
| "E" | earlier document published on or after the international filing date | "Y" | document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art |
| "L" | document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) | "&" | document member of the same patent family |
| "O" | document referring to an oral disclosure, use, exhibition or other means | | |
| "P" | document published prior to the international filing date but later than the priority date claimed | | |

| | |
|---|---|
| Date of the actual completion of the international search<br>01 SEPTEMBER 1994 | Date of mailing of the international search report<br>13 SEP 1994 |
| Name and mailing address of the ISA/US<br>Commissioner of Patents and Trademarks<br>Box PCT<br>Washington, D.C. 20231<br>Facsimile No. (703) 305-3230 | Authorized officer<br>H. Sidberry<br>Telephone No. (703) 308-0196 |

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| Y | The Journal of Immunology, Volume 150, No. 2, issued 15 January 1993, Boehncke et al., "The Importance of Dominant Negative Effects of Amino Acid Side Chain Substitution in Peptide-MHC Molecule Interactions and T Cell Recognition", pages 331-341, see Abstract, on page 331. | 8-11 |
| X | The EMBO Journal, Volume 9, No. 6, issued 1990, Jardetzky et al., "Peptide binding to HLA-DR1: a Peptide with most residues substituted to alanine retains MHC binding", pages 1797-1803, see page 1798, page 1800, figure 4, and page 1801, figure 7. | 5--12 |
| Y | Nature, Volume 332, issued 28 April 1988, Brown et al., "A hypothetical model of the foreign antigen binding site of Class II histocompatibility molecules", pages 845-850, see pages 845-849. | 1, 3, 4 |

# INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

**Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)**

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims Nos.: 2
because they relate to subject matter not required to be searched by this Authority, namely:

Claim 2 is directed to a computerized model which encompasses scientific theory and computer programs to the extent that the International Searching Authority is not equipped to search prior art concerning such programs. Accordingly claim 2 is withdrawn from search under PCT Rule 39 and PCT Article 17(2)(a)(i).

2. [ ] Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. [ ] Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

**Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)**

This International Searching Authority found multiple inventions in this international application, as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. [ ] As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. [ ] No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

**Remark on Protest**

[ ] The additional search fees were accompanied by the applicant's protest.

[ ] No protest accompanied the payment of additional search fees.